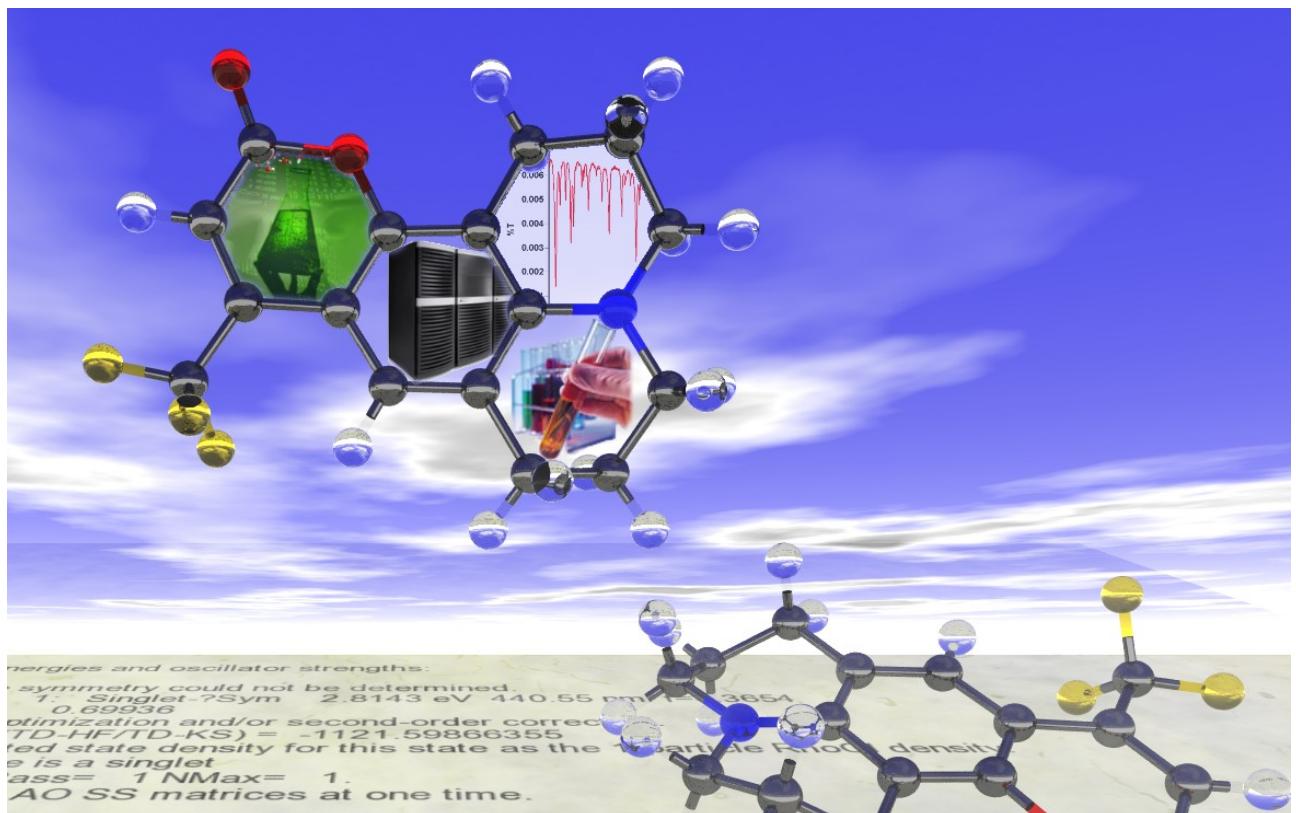


Publication List

Professor Vincenzo Barone

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Scuola Normale Superiore

Selected chapters in collective volumes

- V. Barone, C. Puzzarini, “Interpretability meets Accuracy in Computational Spectroscopy: The Virtual Multifrequency Spectrometer” in *Molecular Spectroscopy: A Quantum Chemistry Approach*, M. Wojcik, Y. Ozaki, J. Popp Eds., 2019, in press.
- D. Licari, G. Mancini, A. Brogni, A. Salvadori, V. Barone, “The SMART Cyberinfrastructure: Space-Time Multiscale Approaches for Research and Technology” in *Computational Chemistry Methodology in Structural Biology and Materials Sciences*, T. Chakraborty, P. Ranjan and A. Pandey Eds., CRC Press, 2017.
- V. Barone, J.A. Gyamfi, A. Piserchia, “Status and perspectives of a virtual multifrequency spectrometer for ESR” in *Electronic Paramagnetic Resonance*, The Royal Society of Chemistry, 2017.
- V. Barone, E. Benassi, I. Carnimeo, “Computational Spectroscopy in Solution: Methods and Models for investigating Complex Systems” in *Quantum Modeling of Complex Molecular Systems*, J.-L. Rivail, M. Ruiz-Lopez, X. Assfeld Eds., Springer, 2015.
- V. Barone, M. Biczysko, I. Carnimeo, “Computational Tools for Structure, Spectroscopy and Thermochemistry” in *Understanding Organometallic Reaction Mechanisms and Catalysis*, V.P. Ananikov, Ed., Wiley-VCH, 2015.
- V. Barone, Ed. *Computational Strategies for Spectroscopy: From Small Molecules to Nano Systems*, John Wiley & Sons, 2012.
- V. Barone, M. Biczysko, P. Cimino. “Interplay of Stereoelectronic Vibrational and Environmental Effects in Tuning Physicochemical Properties of Carbon-Centered Radicals”. In *Carbon-Centered Free Radicals and Radical Cations*, M. D. E. Forbes, Ed., John Wiley & Sons, 2010, pag. 105-139.
- V. Barone, M. Biczysko, G. Brancato. “Extending the Range of Computational Spectroscopy by QM/MM Approaches. Time-dependent and Time-independent routes”. In *Combining Quantum Mechanics and Molecular Mechanics. Some Recent Progresses in QM/MM*, J. Sabin, S. Canuto, Eds., Advances in Quantum Chemistry Vol. 59. Academic Press, 2010, pag. 17-56.
- V. Barone, A. Polimeni, “The virtual electron paramagnetic resonance laboratory: a user guide to ab initio modeling”. In *Electron Paramagnetic Resonance. A practitioner’s toolkit*, M. Brustolon, E. Giamello Eds., John Wiley & Sons 2009, pag. 251-284.
- V. Barone, G. Brancato, R. Improta, “Toward an integrated computational approach for the description of localized physico-chemical properties involving biomolecules”. In *Computational Proteomics*, M. J. Ramos, Ed., Transworld Research, 2008, pag. 1-24.
- V. Barone, P. Cimino, M. Pavone. “EPR spectra of organic free radicals in solution from an integrated computational approach”. In *Continuum Solvation Models in Chemical Physics*, B. Mennucci, R. Cammi, Eds., John Wiley & Sons, 2007, pag. 145-16.

2019

- [19.1] A. Gambi, A. Pietropolli Charmet, P. Stoppa, N. Tasinato, G. Ceselin, V. Barone, *Molecular synthons for accurate structural determinations: the equilibrium geometry of 1-chloro-1-fluoroethene*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **21**, 3431-3439 (2019), DOI: 10.1039/c8cp04888f.
- [19.2] C. Puzzarini, N. Tasinato, J. Bloino, L. Spada, V. Barone, *State-of-the-art computation of the rotational and IR spectra of the methyl-cyclopropyl cation: hints on its detection in space*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **21**, 3615-3625 (2019), DOI: 10.1039/c8cp04629h.
- [19.3] B. Chandramouli, S. Del Galdo, G. Mancini, V. Barone, *Mechanistic insights into metal ions transit through threefold ferritin channel*, BIOCHIMICA ET BIOPHYSICA ACTA-GENERAL SUBJECTS **1863**, 472-480 (2019), DOI: 10.1016/j.bbagen.2018.11.010.
- [19.4] A. Baiardi, C. J. Stein, V. Barone, M. Reiher, Optimization of highly excited matrix product states with an application to vibrational spectroscopy, JOURNAL OF CHEMICAL PHYSICS **150**, 094113 (2019), DOI: 10.1063/1.5068747.
- [19.5] T. Giovannini, P. Lafiosca, B. Chandramouli, V. Barone, C. Cappelli, Effective yet reliable computation of hyperfine coupling constants in solution by a QM/MM approach: interplay between electrostatics and non-electrostatic effects, JOURNAL OF CHEMICAL PHYSICS **150**, 124102 (2019), DOI: 10.1063/1.5080810.
- [19.6] Z. Saita, A. M. Kosmas, O. N. Ventura, V. Barone, Computational Evidence Suggests That 1-Chloroethanol May Be an Intermediate in the Thermal Decomposition of 2-Chloroethanol into Acetaldehyde and HCl, JOURNAL OF PHYSICAL CHEMISTRY A **123**, 1983-1998 (2019), DOI: 10.1021/acs.jpca.8b11966.
- [19.7] C. Puzzarini, J. Bloino, N. Tasinato and V. Barone, Accuracy and Interpretability: The Devil and the Holy Grail. New Routes Across Old Boundaries in Computational Spectroscopy, CHEMICAL REVIEWS **119**, 8131-8191 (2019).
- [19.8] A. Patti, S. Pedotti, G. Mazzeo, G. Longhi, S. Abbate, L. Paoloni, J. Bloino, M. Fusè, S. Rampino, V. Barone, Ferrocenes with simple chiral substituents: an in depth theoretical and experimental VCD and ECD study, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **21**, 9419-9432 (2019). DOI: 10.1039/c9cp00437h.
- [19.9] S. Del Galdo, B. Chandramouli, G. Mancini, V. Barone, Assessment of multiscale approaches for computing UV-vis spectra in condensed phases: towards an effective yet reliable integration of variational and perturbative QM/MM approaches, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **15**, 3170-3184 (2019), DOI: 10.1021/acs.jctc.9b00120.

2018

- [18.1] C. Puzzarini, V. Barone, *Diving for Accurate Structures in the Ocean of Molecular Systems with the Help of Spectroscopy and Quantum Chemistry*, ACCOUNTS OF CHEMICAL RESEARCH **51**, 548-556 (2018), DOI: 10.1021/acs.accounts.7b00603.
- [18.2] F. Fracchia, G. Del Frate, G. Mancini, W. Rocchia, V. Barone, *Force Field Parametrization of Metal Ions from Statistical Learning Techniques*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **14**, 255–273 (2018), DOI: 10.1021/acs.jctc.7b00779.
- [18.3] P. Manini, M. Bietti, M. Galeotti, M. Salamone, O. Lanzalunga, M. M. Cecchini, S. Reale, O. Crescenzi, A. Napolitano, F. De Angelis, V. Barone, M. d'Ischia, *Characterization and Fate of Hydrogen-Bonded Free-Radical Intermediates and Their Coupling Products from the Hydrogen Atom Transfer Agent 1,8-Naphthalenediol*, ACS OMEGA **3**, 3918–3927 (2018), DOI: 10.1021/acsomega.8b00155.
- [18.4] B. Chandramouli, S. Del Galdo, G. Mancini, N. Tasinato, V. Barone, *Tailor-made computational protocols for precise characterization of small biological building blocks using QM and MM approaches*, BIOPOLYMERS **109**, e23109 (2018), DOI: 10.1002/bip.23109.
- [18.5] E. Schiavo, C. Latouche, V. Barone, O. Crescenzi, A B. Muñoz Garcia, M. Pavone, *An ab-initio study of Cu-based delafossites as an alternative to nickel oxide in photocathodes: effects of Mg-doping and surface electronic features*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **20**, 14082-14089 (2018), DOI: 10.1039/C8CP00848E.
- [18.6] P. Cimino, A. Troiani, F. Pepi, S. Garzoli, C. Salvini, B. Di Renzo, V. Barone, A. Ricci, *From Ascorbic Acid to Furan Derivatives: the Gas Phase Acid Catalyzed Degradation of Vitamin C*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **20** (2018), DOI: 10.1039/C8CP01893F.
- [18.7] A. Melli, M. Melosso, N. Tasinato, G. Bosi, L. Spada, J. Bloino, M. Mendolicchio, L. Dore, V. Barone, C. Puzzarini, *Rotational and Infrared Spectroscopy of Ethanamine: A Route toward Its Astrophysical and Planetary Detection*, THE ASTROPHYSICAL JOURNAL **855**, 123 (2018). DOI: 10.3847/1538-4357/aaa899.
- [18.8] F. Egidi, M. Fusè, A. Baiardi, J. Bloino, X. Li, V. Barone, *Computational simulation of vibrationally resolved spectra for spin-forbidden transitions*, CHIRALITY **30**, 850–865 (2018), DOI: 10.1002/chir.22864.
- [18.9] J.A. Gyamfi, V. Barone, *On the composition of an arbitrary collection of SU (2) spins: an enumerative combinatoric approach*, JOURNAL OF PHYSICS A **51**, 105202 (2018), DOI: 10.1088/1751-8121/aaa8fa.
- [18.10] M. Fusé, I. Rimoldi, G. Facchetti, S. Rampino, V. Barone, *Exploiting coordination geometry to selectively predict the sigma-donor and pi-acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy*, CHEMICAL COMMUNICATIONS **54**, 2397-2400 (2018), DOI: 10.1039/C7CC09627E.
- [18.11] M. Macchiagodena, G. Mancini, M. Pagliai, G. Cardini, V. Barone, *New atomistic model of pyrrole with improved liquid state properties and structure*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **118**, spec. Iss. SI, Article Number e25554 (2018), DOI: 10.1002/qua.25554.

[18.12] D. Skouteris, N. Balucani, C. Ceccarelli, F. Vazart, C. Puzzarini, V. Barone, C. Codella, B. Lefloch, *The genealogical tree of ethanol: gas-phase formation of glycolaldehyde, acetic acid, and formic acid*, ASTROPHYSICAL JOURNAL **854**, Article number 135 (2018), DOI:10.3847/1538-4357/aaa41e.

[18.13] M. Melosso, A. Melli, C. Puzzarini, C. Codella, L. Spada, L. Dore, C. Degli Esposti, B. Lefloch, R. Bachiller, C. Ceccarelli, J. Cernicharo, V. Barone, *Laboratory measurements and astronomical search for cyanomethanimine*, ASTRONOMY&ASTROPHYSICS **602**, Article number A121 (2018), DOI:10.1051/0004-6361/201731972.

[18.14] E. Schiavo, A. B. Muñoz Garcia, V. Barone, A. Vittadini, M. Casarin, D. Forrer, M. Pavone, *Tuning dispersion correction in DFT-D2 for metal-molecule interactions: a tailored reparametrization strategy for the adsorption of aromatic systems on Ag(111)*, CHEMICAL PHYSICS LETTERS **693**, 28-33 (2018), DOI: 10.1016/j.cplett.2018.01.005.

[18.15] L. Falivene, V. Barone, G. Talarico, *Unraveling the role of entropy in tuning unimolecular vs. bimolecular reaction rates: the case of olefin polymerization catalyzed by transition metals*, MOLECULAR CATALYSIS **452**, 138-144 (2018), DOI: 10.1016/j.mcat.2018.04.012

[18.16] G. Marianetti, M. Lessi, V. Barone, F. Bellina, A. Pucci, P. Minei, *Solar collectors based on luminescent 2,5-diarylimidazoles*, DYES AND PIGMENTS **157**, 334-341 (2018), DOI: 10.1016/j.dyepig.2018.04.062.

[18.17] T. Fornaro, J.R. Brucato, C. Feuille, D.A. Sverjensky, R.H. Azen, R. Brunetto, M. D'Amore, V. Barone, *Binding of nucleic acid components to the serpentine-hosted hydrothermal mineral brucite*, ASTROBIOLOGY **18**, 1-19 (2018), DOI: 10.1089/ast.2017.1784

[18.18] V. Barone, I. Cacelli, A. Ferretti, *The role of the multiconfigurational character of nitronyl-nitroxide in the singlet-triplet energy gap of its diradicals*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **20**, 18547-18555 (2018), DOI: 10.1039/c8cp02165a.

[18.19] L. Zanetti-Polzi, S. Del Galdo, I. Daidone, M. D'Abramo, V. Barone, M. Aschi, A. Amadei, *Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **20**, 24369-24378 (2018), DOI: 10.1039/c8cp04190c.

[18.20] S. Del Galdo, G. Mancini, I. Daidone, L. Zanetti Polzi, A. Amadei, V. Barone, *Tyrosine absorption spectroscopy: Backbone protonation effects on the side chain electronic properties*, JOURNAL OF COMPUTATIONAL CHEMISTRY **39**, 1747-1756 (2018), DOI: 10.1002/jcc.25351.

[18.21] D. Licari, M. Fusè, A. Salvadori, N. Tasinato, M. Mendolicchio, G. Mancini, V. Barone, *Towards the SMART workflow system for computational spectroscopy*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **20**, 26034-26052 (2018), DOI: 10.1039/C8CP03417F.

[18.22] Li, Weixing, Spada, Lorenzo, Tasinato, Nicola, Rampino, Sergio, Evangelisti, Luca, Gualandi, Andrea, Cozzi, Pier Giorgio, Melandri, Sonia, Barone, Vincenzo, Puzzarini, Cristina , Theory Meets Experiment for Noncovalent Complexes: The Puzzling Case of Pnicogen Interactions, ANGEWANDTE CHEMIE. INTERNATIONAL EDITION **57**, 13853-13857, DOI: 10.1002/anie.201807751

[18.23] Obenchain, Daniel A., Spada, Lorenzo, Alessandrini, Silvia, Rampino, Sergio, Herbers, Sven, Tasinato, Nicola, Mendolicchio, Marco, Kraus, Peter, Gauss, Jürgen, Puzzarini, Cristina, GRABOW, Jens-Uwe, Barone, Vincenzo, Unveiling the Sulfur-Sulfur Bridge: Accurate Structural and Energetic Characterization of a Homochalcogen Intermolecular Bond. ANGEWANDTE CHEMIE. INTERNATIONAL EDITION **57**, 15822-15826, DOI: 10.1002/anie.201810637

[18.24] A. Baiardi, J. Bloino, V. Barone, *Time-Dependent Formulation of Resonance Raman Optical Activity Spectroscopy*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **14**, 6370-6390 (2018), DOI: 10.1021/acs.jctc.8b00488.

[18.25] S. Potenti, P. Manini, T. Fornaro, G. Poggiali, O. Crescenzi, A. Napolitano, J.R. Brucato, V. Barone, M. d'Ischia, *Solid State Photochemistry of Hydroxylated Naphthalenes on Minerals: Probing Polycyclic Aromatic Hydrocarbon Transformation Pathways under Astrochemically-Relevant Conditions*, ACS EARTH AND SPACE CHEMISTRY **2**, 977-1000 (2018), DOI: 10.1021/acsearthspacechem.8b00060.

2017

- [17.1] A. Piserchia, S. Banerjee, V. Barone, *General Approach to Coupled Reactive Smoluchowski Equations: Integration and Application of Discrete Variable Representation and Generalized Coordinate Methods to Diffusive Problems*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 5900-5910 (2017), DOI: 10.1021/acs.jctc.7b00685.
- [17.2] C. Latouche, J.-H. Liao, Y.-J. Li, Y Shiu, V. Barone, S. Kahlal, C.W. Liu, J.-Y. Saillard, *Encapsulating Iodine and Copper into Copper(I) Clusters Stabilized by Dichalcogenolate Ligands: Stability, Structure, and Optical Properties*, INORGANIC CHEMISTRY **56**, 14135-14146 (2017), doi=10.1021/facs.inorgchem.7b02269.
- [17.3] G. Carrillo-Parramon, S. Del Galdo, M. Aschi, G. Mancini, A. Amadei, V. Barone, *Flexible and Comprehensive Implementation of MD-PMM Approach in a General and Robust Code*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 5506-5514 (2017), DOI: 10.1021/acs.jctc.7b00341.
- [17.4] N. Tasinato, C. Puzzarini, V. Barone, *Correct Modeling of Cisplatin: a Paradigmatic Case*, ANGEWANDTE CHEMIE - INTERNATIONAL EDITION **56**, 13838-13841 (2017), DOI: 10.1002/anie.201707683.
- [17.5] D. Licari, N. Tasinato, L. Spada, C. Puzzarini, V. Barone, *VMS-ROT: A New Module of the Virtual Multifrequency Spectrometer for Simulation, Interpretation, and Fitting of Rotational Spectra*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 4382-4396 (2017), DOI: 10.1021/acs.jctc.7b00533
- [17.6] C. Puzzarini, A. Baiardi, J. Bloino, V. Barone, T.E. Murphy, H.D. Drew, H.D., A. Ali, *Spectroscopic Characterization of Key Aromatic and Heterocyclic Molecules: A Route toward the Origin of Life*, ASTRONOMICAL JOURNAL **154** (3), art. no. 82 (2017), . DOI: 10.3847/1538-3881/aa7d54
- [17.7] C. Codella, C. Ceccarelli, P. Caselli, N. Balucani, V. Barone, F. Fontani, B. Lefloch, L. Podio, S. Viti, S. Feng, R. Bachiller, E., Bianchi, F. Dulieu, I. Jiménez-Serra, J. Holdship, R. Neri, J.E. Pineda, A Pon, I. Sims, S. Spezzano, A.I. Vasyunin, F. Alves, L. Bizzocchi, S. Bottinelli, E. Caux, A. Chacón-Ta., R. Choudhury, A. Coutens, C. Favre, P. Hily-Blant, C. Kahane, A. Jaber Al-Edhari, J. Laas, A. López-Sepulcre, J. Ospina, Y. Oya, A. Punanova, C. Puzzarini, D. Quenard, A. Rimola, N. Sakai, D. Skouteris, V. Taquet, L. Testi, P. Theulé, P. Ugliengo, C. Vastel, F. Vazart, L. Wiesenfeld, S. Yamamoto, *Seeds of Life in Space (SOLIS): II. Formamide in protostellar shocks: Evidence for gas-phase formation*, ASTRONOMY AND ASTROPHYSICS **605**, art. no. L3, (2017), DOI: 10.1051/0004-6361/201731249
- [17.8] A. Baiardi, C.J. Stein, V. Barone, V., M. Reiher, *Vibrational Density Matrix Renormalization Group*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 3764-3777 (2017), DOI: 10.1021/acs.jctc.7b00329
- [17.9] A. Baiardi, L. Paoloni, V. Barone, V.G. Zakrzewski, J.V. Ortiz, *Assessment of Electron Propagator Methods for the Simulation of vibrationally Resolved Valence and Core Photoionization Spectra*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 3120-3135 (2017), DOI: 10.1021/acs.jctc.6b00958.

[17.10] L. Spada, N. Tasinato, G. Bosi, F. Vazart, V. Barone, C. Puzzarini, *On the competition between weak O–H···F and C–H···F hydrogen bonds, in cooperation with C–H···O contacts, in the difluoromethane – tert-butyl alcohol cluster*, JOURNAL OF MOLECULAR SPECTROSCOPY **337**, 90-95 (2017), DOI: 10.1016/j.jms.2017.04.001.

[17.11] A. Baiardi, J. Bloino, V. Barone, *Simulation of Vibronic Spectra of Flexible Systems: Hybrid DVR-Harmonic Approaches*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 2804-2822 (2017), DOI: 10.1021/acs.jctc.7b00236.

[17.12] M. Mendolicchio, E. Penocchio, D. Licari, N. Tasinato, V. Barone, *Development and Implementation of Advanced Fitting Methods for the Calculation of Accurate Molecular Structures*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **13**, 3060-3075 (2017), DOI: 10.1021/acs.jctc.7b00279.

[17.13] F. Egidi, D.B. Williams-Young, A. Baiardi, J. Bloino, G. Scalmani, M.J. Frisch, X. Li, V Barone, *Effective Inclusion of Mechanical and Electrical Anharmonicity in Excited Electronic States: VPT2-TDDFT Route*, Journal of Chemical Theory and Computation **13**, 2789-2803 (2017), DOI: 10.1021/acs.jctc.7b00218.

[17.14] Presti, D., Pedone, A., Licari, D., Barone, V., *A Modular Implementation for the Simulation of 1D and 2D Solid-State NMR Spectra of Quadrupolar Nuclei in the Virtual Multifrequency Spectrometer-Draw Graphical Interface*, Journal of Chemical Theory and Computation **13**, 2215-2229 (2017), DOI: 10.1021/acs.jctc.7b00154.

[17.15] A. Pedone, F. Palazzetti, V. Barone, *Models of Aged Magnesium-Silicate-Hydrate Cements Based on the Lizardite and Talc Crystals: A Periodic DFT-GIPAW Investigation*, JOURNAL OF PHYSICAL CHEMISTRY C **121**, 7319-7330 (2017). DOI: 10.1021/acs.jpcc.7b00708

[17.16] L. Evangelisti, L., Spada, W. Li, F. Vazart, V. Barone, W. Caminati, *The Borderline between Reactivity and Pre-reactivity of Binary Mixtures of Gaseous Carboxylic Acids and Alcohols*, (2017) ANGEWANDTE CHEMIE - INTERNATIONAL EDITION **56**, 3872-3875 (2017), DOI: 10.1002/anie.201612231.

[17.17] M. Macchiagodena, G. Del Frate, G. Brancato, B. Chandramouli, G. Mancini, V. Barone, *Computational study of the DPAP molecular rotor in various environments: From force field development to molecular dynamics simulations and spectroscopic calculations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **19**, 30590-30602 (2017), DOI: 10.1039/c7cp04688j.

[17.18] M. Macchiagodena, G. Mancini, M. Pagliai, G. Del Frate, V. Barone, *Fine-tuning of atomic point charges: Classical simulations of pyridine in different environments*, CHEMICAL PHYSICS LETTERS, **677**, 120-126 (2017), DOI: 10.1016/j.cplett.2017.04.004.

[17.19] M. Fusè, I. Rimoldi, E. Cesarotti, S. Rampino, V. Barone, *On the relation between carbonyl stretching frequencies and the donor power of chelating diphosphines in nickel dicarbonyl complexes*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **19**, 9028-9038 (2017), DOI: 10.1039/c7cp00982h.

[17.20] V. Barone, J.A. Gyamfi, A. Pischedda, *Status and perspectives of a virtual multifrequency spectrometer for ESR*, ELECTRON PARAMAGNETIC RESONANCE **25**, 98-156 (2017), DOI: 10.1039/9781782629436-00098.

[17.21] V. Barone, I. Cacelli, A. Ferretti, G. Prampolini, *Quantitative prediction and interpretation of spin energy gaps in polyradicals: The virtual magnetic balance*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **19**, 9039-9044 (2017), DOI: 10.1039/c7cp00186j.

[17.22] S. Banerjee, D. Skouteris, V. Barone, *A diabatic electronic state system to describe the internal conversion of azulene*, LECTURE NOTES IN COMPUTER SCIENCE **10408 LNCS**, 328-337 (2017), DOI: 10.1007/978-3-319-62404-4_24.

[17.23] M. Pagliai, G. Mancini, I. Carnimeo, N. De Mitri, V. Barone, *Electronic absorption spectra of pyridine and nicotine in aqueous solution with a combined molecular dynamics and polarizable QM/MM approach*, JOURNAL OF COMPUTATIONAL CHEMISTRY **38**, 319-335 (2017), DOI: 10.1002/jcc.24683.

[17.24] Barone, V., Cacelli, I., Ferretti, A., Prampolini, G., *Magnetic gaps in organic tri-radicals: From a simple model to accurate estimates*, JOURNAL OF CHEMICAL PHYSICS **146**, 104103, DOI: 10.1063/1.4977598.

[17.25] L. Spada, N. Tasinato, F. Vazart, V. Barone, W. Caminati, C. Puzzarini, *Noncovalent Interactions and Internal Dynamics in Pyridine-Ammonia: A Combined Quantum-Chemical and Microwave Spectroscopy Study*, CHEMISTRY - A EUROPEAN JOURNAL **23**, 4876-4883 (2017), DOI: 10.1002/chem.201606014

2016

- [16.1] B. Carlotti, E.Benassi, C.Fortuna, V.Barone, A.Spalletti, F.Elisei, *Efficient excited state symmetry breaking in a cationic quadrupolar system bearing diphenylamino donors*, CHEMPHYSCHM **17**, 136-146 (2016), DOI: 10.1002/cphc.201500784.
- [16.2] D. Presti, A. Pedone, G. Mancini, C. Duce, M. Tinè, V. Barone, *Insights on structural and dynamical features of water at halloysite interfaces probed by DFT and classical Molecular Dynamics simulations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **18**, 2164-2174 (2016), DOI: 10.1039/C5CP05920H
- [16.3] V. Barone, *The Virtual Multifrequency Spectrometer: a New Paradigm for Spectroscopy*, WIRES COMPUTATIONAL MOLECULAR SCIENCES **6**, 86-110 (2016), DOI: 10.1002/wcms.1238.
- [16.4] P. Minei, M. Ahmad, V. Barone, G. Brancato, E. Passaglia, G. Bottari, A. Pucci, *Vapochromic behaviour of polycarbonate films doped with a luminescent molecular rotor*, POLYMERS FOR ADVANCED TECHNOLOGIES **27**, 429-435 (2016), DOI: 10.1002/pat.3688.
- [16.5] D. Skouteris, D. Calderini, V. Barone, *Methods for calculating partition functions of molecules involving large amplitude and/or anharmonic motions*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **12**, 1011-1018 (2016), DOI: 10.1021/acs.jctc.5b01094.
- [16.6] S. Banerjee, A. Baiardi, J. Bloino, V. Barone, *Temperature dependence of radiative and non-radiative rates from time-dependent correlation function methods*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **12**, 774-786 (2016), DOI: 10.1021/acs.jctc.5b01017.
- [16.7] A. Baiardi, J. Bloino, V. Barone, *General formulation of vibronic spectroscopy in internal coordinates*, JOURNAL OF CHEMICAL PHYSICS **144**, 084114 (2016), DOI: 10.1063/1.4942165.
- [16.8] J. Meinnel, C. Latouche, S. Ghanami, A. Boucekkine, V. Barone, A. Moreac, A. Boudjada, *Anharmonic computations meet experiment (IR, Raman, Neutron diffraction) for 1,3,5-tribromo-2,4,6-trimethylbenzene*, JOURNAL OF PHYSICAL CHEMISTRY A **120**, 1127-1132 (2016), DOI: 10.1021/acs.jpca.5b12467
- [16.9] T. Fornaro, M.Biczysko, V. Barone, *Reliable vibrational wavenumbers for C=O and N-H stretchings of isolated and hydrogen-bonded nucleic acid bases*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **18**, 8479-8490 (2016), DOI: 10.1039/C5CP07386C.
- [16.10] G.Del Frate, F.Bellina, G.Mancini, G.Marianetti, P.Minei, A.Pucci, V. Barone, *Tuning of dye optical properties by environmental effects: a QM/MM and experimental study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **18**, 9724-9733 (2016), DOI: 10.1039/C6CP00841K.
- [16.11] F. Vazart, P. Savel, C. Latouche, V. Barone, F.Camerel, T.Roisnel, J.-L.Fillaut, H.Akdas-Kilig, M.Achard, *Neutral copper(I) complexes featuring phosphinesulfonate chelates*, DALTON TRANSACTIONS **45**, 6566-6573 (2016), DOI:10.1039/C6DT00593D.

[16.12] M. Hodecker, M. Biczysko, A. Drew, V. Barone, *Simulation of vacuum UV absorption and electronic circular dichroism spectra of methyl oxirane: the role of vibrational effects*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **12**, 2820-2833 (2016), DOI: 10.1021/acs.jctc.6b00121.

[16.13] S. Banerjee, A. Baiardi, J. Bloino, V. Barone, *Vibronic effects on rates of excitation energy transfer and their temperature dependence*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **12**, 2357-2365 (2016), DOI: 10.1021/acs.jctc.6b00157.

[16.14] S. Grubisic, B. Chandramouli, V. Barone, G. Brancato, *Chain length, temperature and solvent effects on the structural properties of α -aminoisobutyric acid homooligopeptides*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **18**, 20389-20398 (2016), DOI: 10.1039/C5CP07386C.

[16.15] F. Massuyeau, E. Faulques, C. Latouche, V. Barone, *New insights in the vibrational and optical signatures of trans-stilbene via integrated experimental and quantum mechanical approaches*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **18**, 19378-19385 (2016), DOI: 10.1039/C6CP02787C.

[16.16] M. Piccardo, E. Penocchio, C. Puzzarini, M. Biczysko, V. Barone, *Erratum: Semi-Experimental Equilibrium Structure Determinations by Employing B3LYP/SNSD Anharmonic Force Fields: Validation and Application to Semirigid Organic Molecules*, Journal of Physical Chemistry A **119** (2058-2082) 2015, DOI: 10.1021/jp511432m): JOURNAL OF PHYSICAL CHEMISTRY A, **120**, 3754 (2016), DOI: 10.1021/acs.jpca.6b04648

[16.17] A. Piserchia, V. Barone, *Toward a General Yet Effective Computational Approach for Diffusive Problems: Variable Diffusion Tensor and DVR Solution of the Smoluchowski Equation along a General One-Dimensional Coordinate*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **12**, 3482-3490 (2016), DOI: 10.1021/acs.jctc.6b00388

[16.18] F.A. Gianturco, M. Satta, M., Mendolicchio, F. Palazzetti, A. Piserchia, V. Barone, R. Wester, *Exploring a chemical route for the formation of stable anions of polyynes [C_nH_n] (n = 2, 4)] in molecular clouds*, ASTROPHYSICAL JOURNAL, 830 (1), art. no. 2 (2016), DOI: 10.3847/0004-637X/830/1/2.

[16.19] F. Bellina, C. Manzini, G. Marianetti, C. Pezzetta, E. Fanizza, M. Lessi, P. Minei, V. Barone, A. Pucci, *Colourless p-phenylene-spaced bis-azoles for luminescent concentrators*, DYES AND PIGMENTS **134**, 118-128 (2016), DOI: 10.1016/j.dyepig.2016.07.005.

[16.20] V. Barone, *Theoretical and computational chemistry in Italy*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **116**, 1499-1500 (2016), DOI: 10.1002/qua.25291.

[16.21] F. Vazart, D. Calderini, C. Puzzarini, D. Skouteris, V. Barone, *State-of-the-Art Thermochemical and Kinetic Computations for Astrochemical Complex Organic Molecules: Formamide Formation in Cold Interstellar Clouds as a Case Study*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **12**, 5385-5397 (2016), DOI: 10.1021/acs.jctc.6b00379

[16.22] A. Salvadori, G. Del Frate, M. Pagliai, G. Mancini, V. Barone, *Immersive virtual reality in computational chemistry: Applications to the analysis of QM and MM data*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **116**, 1731-1746 (2016), DOI: 10.1002/qua.25207.

[16.23] A. Ricci, F. Pepi, P. Cimino, A. Troiani, S. Garzoli, C. Salvitti, B. Di Rienzo, V. Barone, *Vitamin C: an experimental and theoretical study on the gas-phase structure and ion energetics of protonated ascorbic acid*, JOURNAL OF MASS SPECTROMETRY **51**, 1146-1151 (2016), DOI: 10.1002/jms.3848.

[16.24] F. Egidi, F. Trani, P.A. Ballone, V. Barone, W. Andreoni, W., *Low-lying electronic excitations of a water-soluble BODIPY: from the gas phase to the solvated molecule*, THEORETICAL CHEMISTRY ACCOUNTS **135**, art. no. 264 (2016), DOI: 10.1007/s00214-016-2011-9.

2015

- [15.01] C. Latouche, H. Akdas-Kilig, J.-P. Malval, J.-L. Fillaut, A. Boucekkine, V. Barone, *Theoretical Evidence of Metal-Induced Structural Distortions in a Series of Bipyrimidine-Based Ligands*, DALTON TRANSACTIONS **44**, 506-510 (2015), DOI:10.1039/C4DT03291H.
- [15.02] D. Licari, A. Baiardi, M. Biczysko, F. Egidi, C. Latouche, V. Barone, *Implementation of a graphic user interface for the virtual multifrequency spectrometer: the VMS-Draw tool*, JOURNAL OF COMPUTATIONAL CHEMISTRY **36**, 321-334 (2015), DOI: 10.1002/jcc.23785.
- [15.03] C. Latouche, A. Baiardi, V. Barone, *Virtual eyes designed for quantitative spectroscopy of inorganic complexes: vibronic signatures in the phosphorescence spectra of terpyridine derivatives*, JOURNAL OF PHYSICAL CHEMISTRY B **24**, 7253-7257 (2015), DOI: 10.1021/jp510589u
- [15.04] E. Benassi, B. Carlotti, C. Fortuna, V. Barone, F. Elisei, A. Spalletti, *Acid–Base Strength and Acidochromism of Some Dimethylamino–Azinium Iodides. An Integrated Experimental and Theoretical Study*, JOURNAL OF PHYSICAL CHEMISTRY A **119**, 323-333 (2015), DOI 10.1021/jp510982h.
- [15.05] E. Benassi, F. Egidi, V. Barone, *General strategy for computing nonlinear optical properties of large neutral and cationic organic chromophores in solution*, JOURNAL OF PHYSICAL CHEMISTRY B **119**, 3155-3173 (2015) DOI 10.1021/jp512342y.
- [15.06] R. Impronta, V. Barone, *Excited States behavior of nucleobases in solution: insights from computational studies*, TOPICS IN CURRENT CHEMISTRY **355**, 329-357 (2015) DOI 10.1007/128_2013_524.
- [15.07] M. Piccardo, E. Penocchio, C. Puzzarini, M. Biczysko, V. Barone, *Semi-experimental equilibrium structure determinations by employing B3LYP/SNSD anharmonic force fields: validation and application to semirigid organic molecules*, JOURNAL OF PHYSICAL CHEMISTRY A, **119**, 2058-2082 (2015), DOI: 10.1021/jp511432m.
- [15.08] G. Mancini, G. Brancato, B. Chandramouli, V. Barone, *Organic solvents simulations under non periodic boundary conditions: a library of effective potentials for the GLOB model*, CHEMICAL PHYSICS LETTERS, **625**, 186-192 (2015), DOI:10.1016/j.cplett.2015.03.001.
- [15.09] B. Chandramouli, D. Di Maio, G. Mancini, G. Brancato, V. Barone, *Breaking the Hydrophobicity of the MscL Pore: Insights into a Charge-Induced Gating Mechanism*, PLOS ONE, **10**, e0120196 (2015), DOI 10.1371/journal.pone.0120196.
- [15.10] F. Vazart, D.Calderini, D.Skouteris, C.Latouche, V.Barone, *Re-Assessment of the Thermodynamic, Kinetic, and Spectroscopic Features of Cyanomethanimine Derivatives: A Full Anharmonic Perturbative Treatment*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **11**,1165-1171 (2015), DOI: 10.1021/ct501147a.
- [15.11] L.N. Vidal, F. Egidi, V. Barone, C. Cappelli, *Origin invariance in vibrational resonance Raman optical activity*, JOURNAL OF CHEMICAL PHYSICS **142**, 174101 (2015), DOI: 10.1063/1.4918935.

[15.12] T. Fornaro, D. Burini, M. Biczysko, V. Barone, *Hydrogen-bonding effects on infrared spectra from anharmonic computations: uracil-water complexes and uracil dimers*, JOURNAL OF PHYSICAL CHEMISTRY A, **119**, 4224-4236 (2015).

[15.13] E. Benassi, B. Carlotti, M. Segado, A. Cesaretti, A. Spalletti, F. Elisei, V. Barone, *Presence of two emissive minima in the lowest excited state of a push-pull cationic dye unequivocally proved by femtosecond up-conversion spectroscopy and vibronic quantum-mechanical computations*, JOURNAL OF PHYSICAL CHEMISTRY B, **119**, 6035-6040 (2015) DOI: 10.1021/acs.jpcb.5b03545.

[15.14] I. Cacelli, A. Ferretti, G. Prampolini, V. Barone, *BALOO: a Fast and Versatile Code for Accurate Multi-Reference Variational/Perturbative Calculations* JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 2024-2035 (2015) DOI:10.1021/ct501071k.

[15.15] B. Carlotti, E. Benassi, V. Barone, G. Consiglio, F. Elisei, A. Mazzoli, A. Spalletti, *Effect of the π -bridge and the acceptor on the intramolecular charge transfer in push-pull cationic chromophores: a joint ultrafast spectroscopic and TD-DFT computational study*, CHEMPHYSCHM **16**, 1440-1450 (2015) DOI:10.1002/cphc.201402896.

[15.16] F. Vazart, C. Latouche, J. Bloino, V. Barone, *Vibronic coupling investigation to compute phosphorescence spectra of Pt(II) complexes*, INORGANIC CHEMISTRY **54**, 5588-5595 (2015) DOI:10.1021/acs.inorgchem.5b00734.

[15.17] V. Barone, M. Biczysko, C. Puzzarini, *Quantum chemistry meets spectroscopy for astrochemistry: increasing complexity toward prebiotic molecules*, ACCOUNTS OF CHEMICAL RESEARCH **48**, 1413-1422 (2015) DOI:10.1021/ar5003285.

[15.18] G. Brancato, G. Signore, P. Neyroz, D. Polli, G. Cerullo, G. Abbandonato, L. Nucara, V. Barone, F. Beltram, R. Bizzarri, *Dual fluorescence through Kasha's rule breaking: an unconventional photomechanism for intracellular probe design*, JOURNAL PHYSICAL CHEMISTRY B **119**, 6144-6154 (2015) DOI:10.1021/acs.jpcb.5b01119.

[15.19] M. Piccardo, J. Bloino, V. Barone, *Generalized vibrational perturbation theory for rotovibrational energies of linear, symmetric, and asymmetric tops: theory, approximations, and automated approaches to deal with medium-to-large molecular systems*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **115**, 948-982 (2015), DOI:10.1002/qua.24931

[15.20] P. Manini, V. Criscuolo, L. Ricciotti, A. Pezzella, M. Barra, A. Cassinese, O. Crescenzi, M.G. Maglione, P. Tassini, C. Minarini, V. Barone, M. d'Ischia, *Melanin-inspired organic electronics: electroluminescence in asymmetric triazatruxenes*, CHEMPLUSCHEM **80**, 919-927 (2015), DOI: 10.1002/cplu.201402444.

[15.21] A. Piserchia, V. Barone, *Discrete variable representation of Smoluchowski equation using a sinc basis set*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **17**, 17362-17374 (2015) DOI:10.1039/C5CP02060C.

[15.22] A. Baiardi, J. Bloino, V. Barone, *Accurate simulation of resonance-raman spectra of flexible molecules: an internal coordinates approach*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 3267-3280 (2015), DOI:10.1021/acs.jctc.5b00241.

[15.23] C. Latouche, D. Skouteris, F. Palazzetti, V. Barone, *TD-DFT benchmark on inorganic Pt(II) and Ir(III) complexes*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 3281-3289 (2015), DOI: 10.1021/acs.jctc.5b00257.

[15.24] D. Skouteris, V. Barone, *Nonadiabatic photodynamics of phenol on a realistic potential energy surface by a novel multilayer Gaussian MCTDH program*, CHEMICAL PHYSICS LETTERS **636**, 15-21 (2015), DOI: 10.1016/j.cplett.2015.06.065.

[15.25] B. Carlotti, E. Benassi, A. Cesaretti, C.G. Fortuna, A. Spalletti, V. Barone, F. Elisei, *An ultrafast spectroscopic and quantum mechanical investigation of multiple emissions in push-pull pyridinium derivatives bearing different electron donors*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **17**, 20981-20989 (2015), DOI:10.1039/C5CP03207E.

[15.26] E. N. Najbauer, G. Bazsó, R. Apóstolo, R. Fausto, M. Biczysko, V. Barone, G. Tarczay, *Identification of serine conformers by matrix-isolation IR spectroscopy aided by near-infrared laser-induced conformational change, 2D correlation analysis, and quantum mechanical anharmonic computations*, JOURNAL OF PHYSICAL CHEMISTRY B **119**, 10496/10510 (2015), DOI: 10.1021/acs.jpca.5b05768.

[15.27] V. Barone, C. Latouche, D. Skouteris, F. Vazart, N. Balucani, C. Ceccarelli, B. Lefloch, *Gas-phase formation of the prebiotic molecule formamide: insights from new quantum computations*, MONTHLY NOTICES OF THE ROYAL ASTRONOMICAL SOCIETY: LETTERS **453**, L31-L35 (2015), DOI: 10.1093/mnrasl/slv094

[15.28] F. Vazart, C. Latouche, D. Skouteris, N. Balucani, V. Barone, *Cyanomethanimine isomers in cold interstellar clouds: insights from electronic structure and kinetic calculations*, ASTROPHYSICAL JOURNAL **810**, 111 (2015)

[15.29] E. Penocchio, M. Piccardo, V. Barone, *Semiexperimental equilibrium structures for building blocks of organic and biological molecules: the B2PLYP route*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 4342-4363 (2015), DOI:10.1021/acs.jctc.5b00580.

[15.30] I. Carnimeo, C. Cappelli, V. Barone, *Analytical gradients for MP2, double hybrid functionals, and TD-DFT with polarizable embedding described by fluctuating charges*, JOURNAL OF COMPUTATIONAL CHEMISTRY **31**, 2271-2290 (2015), DOI: 10.1002/jcc.24195.

[15.31] F. Vazart, C. Latouche, P. Cimino, V. Barone, *Accurate IR spectra for molecules containing the C≡N moiety by anharmonic computations with the double hybrid B2PLYP density functional*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 4364-4369 (2015), DOI :10.1021/acs.jctc.5b00638.

[15.32] V. Barone, M. Biczysko, J. Bloino, P. Cimino, E. Penocchio, C. Puzzarini, *CC/DFT route toward accurate structures and spectroscopic features for observed and elusive conformers of flexible molecules: pyruvic acid as a case study*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 4342-4363 (2015), DOI: 10.1021/acs.jctc.5b00580.

[15.33] V. Barone, F. Bellina, M. Biczysko, J. Bloino, T. Fornaro, C. Latouche, M. Lessi, G. Marianetti,

P.Minei, A.Panattoni, A.Pucci, *Toward the design of alkynylimidazole fluorophores: computational and experimental characterization of spectroscopic features in solution and in poly(methylmethacrylate)*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **17**, 26710-26723 (2015), DOI: 10.1039/C5CP03047A

[15.34] A.Baiardi, M.Mendolicchio, V.Barone, G.Fronzoni, G.A. Cardenas Jimenez, M.Stener, C.Grazioli, M.de Simone, M.Coreno, *Vibrationally resolved NEXAFS at C and N K-edges of pyridine, 2-fluoropyridine and 2,6-difluoropyridine: a combined experimental and theoretical assessment*, JOURNAL OF CHEMICAL PHYSICS **143**, 204102 (2015), <http://dx.doi.org/10.1063/1.4935715>.

[15.35] M. Segado, E. Benassi, V.Barone, *A twist on the interpretation of the multifluorescence patterns of DASPMI*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **11**, 4803-4813 (2015), DOI: 10.1021/acs.ctc.5b00632.

[15.36] H. Kvapilová, A. Vlček, Jr., V. Barone, M. Biczysko, S. Záliš, *Anharmonicity Effects in IR Spectra of [Re(X)(CO)₃(α -diimine)] (α -diimine = 2,2'-bipyridine or pyridylimidazo[1,5a] pyridine; X = Cl or NCS) Complexes in Ground and Excited Electronic States*, JOURNAL OF PHYSICAL CHEMISTRY A **119**, 10137-10146 (2015). DOI: 10.1021/acs.jpca.5b07585

[15.37] F.Muniz-Miranda, A.Pedone, G.Battistelli, M.Montalti, J.Bloino, V. Barone, *Benchmarking TD-DFT against Vibrationally Resolved Absorption Spectra at Room Temperature: 7-Aminocoumarins as Test Cases*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **11**, 5371-5384 (2015), DOI: 10.1021/acs.jctc.5b00750.

[15.38] J.Bloino, M.Biczysko, V. Barone, *Anharmonic Effects on Vibrational Spectra Intensities: Infrared, Raman, Vibrational Circular Dichroism and Raman Optical Activity*, JOURNAL OF PHYSICAL CHEMISTRY A **119**, 11862-11874 (2015) DOI: 10.1021/acs.jpca.5b10067.

[15.39] V. Barone, M. Biczysko, C. Latouche, A. Pasti, *Virtual eyes for technology and cultural heritage: toward computational strategy for new and old indigo-based dyes*, THEORETICAL CHEMISTRY ACCOUNTS **134**, 1-14 (2015).

2014

- [14.01] V. Barone, I. Cacelli, O. Crescenzi, M. d'Ischia, A. Ferretti, G. Prampolini, G. Villani, *Unraveling the interplay of different contributions to the stability of the quinhydrone dimer*, RSC ADVANCES **4**, 876-885 (2014), DOI: 10.1039/c3ra46191b
- [14.02] V. Barone, M. Biczysko, J. Bloino, *Fully anharmonic IR and Raman spectra of medium-size molecular systems: accuracy and interpretation*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **16**, 1759-1787 (2014), DOI: 10.1039/c3cp53413h
- [14.03] L. Carta, M. Biczysko, J. Bloino, D. Licari, V. Barone, *Environmental and complexation effects on the structures and spectroscopic signatures of organic pigments relevant to cultural heritage: the case of alizarin and alizarin-M(II)/Al(III) complexes*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **16**, 2897-2911 (2014), DOI: 10.1039/c3cp50499a
- [14.04] F. Egidi, J. Bloino, C. Cappelli, V. Barone, *A robust and effective time-independent route to the calculation of resonance Raman spectra of large molecules in condensed phases with the inclusion of Duschinsky, Herzberg-Teller, anharmonic, and environmental effects*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **10**, 346-363 (2014), DOI: 10.1021/ct400932e
- [14.05] C. Greco, G. Moro, L. Bertini, M. Biczysko, V. Barone, U. Cosentino, *Computational investigation on the spectroscopic properties of thiophene based europium β -diketonate complexes*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **10**, 767-777 (2014), DOI: 10.1021/ct400865b
- [14.06] C. Puzzarini, M. Biczysko, J. Bloino, V. Barone, *Accurate spectroscopic characterization of oxirane: a valuable route to its identification in titan's atmosphere and the assignment of unidentified infrared bands*, THE ASTROPHYSICAL JOURNAL **785**: 107 (2014), DOI: 10.1088/0004-637X/785/2/107
- [14.07] C. Puzzarini, M. Biczysko, V. Barone, L. Largo, I. Pena, C. Cabezas, J.L. Alonso, *Accurate characterization of the peptide linkage in the gas phase: a joint quantum-chemistry and rotational spectroscopy study of the glycine dipeptide analogue*, JOURNAL OF PHYSICAL CHEMISTRY LETTERS **5**, 534-540 (2014), DOI: 10.1021/jz402744a
- [14.08] M. Lessi, C. Manzini, P. Minei, L.A. Perego, J. Bloino, F. Egidi, V. Barone, A. Pucci, F. Bellina, *Synthesis and Optical Properties of Imidazole-Based Fluorophores having High Quantum Yields*, CHEMPLUSCHEM **79**, 366-370 (2014), DOI: 10.1002/cplu.201300413
- [14.09] G. Mancini, G. Brancato, V. Barone, *Combining the Fluctuating Charge Method, Non-periodic Boundary Conditions and Meta-dynamics: Aqua Ions as Case Studies*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **10**, 1150-1163 (2014), DOI: 10.1021/ct400988e.
- [14.10] G. Prampolini, S. Monti, N. De Mitri, V. Barone, *Evidence of long lived cages in functionalized polymers: effects on chromophore dynamic and spectroscopic properties*, CHEMICAL PHYSICS LETTERS **601**, 134-138 (2014), DOI: 10.1016/j.cplett.2014.04.001
- [14.11] T. Fornaro, M. Biczysko, S. Monti, V. Barone, *Dispersion corrected DFT approaches for anharmonic vibrational frequency calculations: nucleobases and their dimers*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS (2014), Advance Article, DOI: 10.1039/C3CP54724H.
- [14.12] V. Barone, I. Cacelli, A. Ferretti, M. Vischiarelli, *Electron transport properties of diarylethene photoswitches by a simplified NEGF-DFT approach*, JOURNAL OF PHYSICAL CHEMISTRY B **118**, 4976-4981 (2014), DOI: 10.1021/jp502065c.

[14.13] D. Skouteris, V. Barone, *A new Gaussian MCTDH program: implementation and validation on the vibrational levels of the water and glycine molecules*, JOURNAL OF CHEMICAL PHYSICS **140**, 244104 (2014), DOI: 10.1063/1.4883677.

[14.14] V. Barone, M. Biczysko, J. Bloino, L. Carta, A. Pedone, *Environmental and dynamical effects on the optical properties of molecular systems by time-independent and time-dependent approaches: coumarin derivatives as test cases*, COMPUTATIONAL AND THEORETICAL CHEMISTRY **1037**, 35-48 (2014), DOI: 10.1016/j.comptc.2014.03.027.

[14.15] F. Egidi, T. Giovannini, M. Piccardo, J. Bloino, C. Cappelli, V. Barone, *Stereoelectronic, vibrational, and environmental contributions to polarizabilities of large molecular systems: a feasible anharmonic protocol*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **10**, 2456-2464 (2014), DOI: 10.1021/ct500210z.

[14.16] C. Puzzarini, E. Penocchio, M. Biczysko, V. Barone, *Molecular structure and spectroscopic signatures of acrolein: theory meets experiment*, JOURNAL OF PHYSICAL CHEMISTRY A **118**, 6648-6656 (2014), DOI: 10.1021/jp503672g.

[14.17] B. Carlotti, E. Benassi, A. Spalletti, C. G. Fortuna, F. Elisei, V. Barone, *Photoinduced symmetry-breaking intramolecular charge transfer in a quadrupolar pyridinium derivative*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **16**, 13984-13994 (2014), DOI: 10.1039/c4cp00631c.

[14.18] V. Barone, M. Biczysko, J. Bloino, C. Puzzarini, *Accurate molecular structures and infrared spectra of trans-2,3-dideuterooxirane, methyloxirane, and trans-2,3-dimethyloxirane*, JOURNAL OF CHEMICAL PHYSICS **141**, 034107 (2014), DOI: 10.1063/1.4887357.

[14.19] N. De Mitri, G. Prampolini, S. Monti, V. Barone, *Structural, dynamic and photophysical properties of a fluorescent dye incorporated in an amorphous hydrophobic polymer bundle*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **16**, 16573-16587 (2014), DOI: 10.1039/c4cp01828a.

[14.20] C. Puzzarini, A. Ali, M. Biczysko, V. Barone, *Accurate spectroscopic characterization of protonated oxirane: a potential prebiotic species in Titan's atmosphere*, ASTROPHYSICAL JOURNAL **792**: 118 (2014), DOI: 10.1088 / 0004-637X/792/118.

[14.21] V. Barone, A. Baiardi, J. Bloino, *New developments of a multifrequency virtual spectrometer: stereo-electronic, dynamical, and environmental effects on chiroptical spectra*, CHIRALITY **26**, 228-240 (2014), DOI: 10.1002/chir.22325.

[14.22] A. Baiardi, J. Bloino, V. Barone, *A general time-dependent route to Resonance-Raman spectroscopy including Franck-Condon, Herzberg-Teller and Duschinsky effects*, JOURNAL OF CHEMICAL PHYSICS **141**, 114108 (2014), DOI: 10.1063/1.4895534.

[14.23] M. Koenig, T. Torres, V. Barone, G. Brancato, D. M. Guldi, G. Bottariu, *Ultrasound-induced transformation of fluorescent organic nanoparticles from a molecular rotor into rhomboidal nanocrystals with enhanced emission*, CHEMICAL COMMUNICATIONS **50**, 12955-12958 (2014), DOI: 10.139/c4cc05531d.

[14.24] C. Latouche, F. Palazzetti, D. Skouteris, V. Barone, *High-Accuracy Vibrational Computations for Transition-Metal Complexes Including Anharmonic Corrections: Ferrocene, Ruthenocene, and Osmocene as Test Cases*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **10**, 4565-4573 (2014), DOI: 10.1021/ct5006246.

[14.25] V. Barone, M. Biczysko, M. Borkowska-Panek, J. Bloino, *A Multifrequency Virtual Spectrometer for Complex Bio-Organic Systems: Vibronic and Environmental Effects on the UV/Vis Spectrum of Chlorophyll a*, CHEMPHYSCHM **15**, 3355-3364 (2014), DOI: 10.1002/cphc201402300.

[14.26] P. Minei, M. Koenig, A. Battisti, M. Ahrmad, V. Barone, T. Torres, D. M. Guldí, G. Brancato, G. Bottari, A. Pucci, *Reversible vapochromic response of polymer films doped with a highly emissive molecular rotor*, JOURNAL OF MATERIALS CHEMISTRY C **2**, 9224-9232 (2014), DOI: 10.1039/c4tc01737d.

[14.27] A. Baiardi, C. Latouche, J. Bloino, V. Barone, *Accurate yet feasible computations of resonance Raman spectra for metal complexes in solution: $[\text{Ru}(\text{bpy})_3]^{2+}$ as a case study*, DALTON TRANSACTIONS **43**, 17610 – 17614 (2014), DOI: 10.1039/C4DT02151G.

[14.28] E. Benassi, C. Cappelli, B. Carlotti, V. Barone, *An integrated computational tool to model the broadening of the absorption bands of flexible dyes in solution: cationic chromophores as test cases*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **16**, 26963-26973 (2014), DOI: 10.1039/C4CP03419H.

[14.29] C. Latouche, V. Barone, *Computational Chemistry Meets Experiments for Explaining the Behavior of Bibenzyl: A Thermochemical and Spectroscopic (Infrared, Raman, and NMR) Investigation*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **10**, 5586-5592 (2014), DOI: 10.1021/ct500930b.

[14.30] F. Egidi, M. Segado, H. Koch, C. Cappelli, V. Barone, *A benchmark study of electronic excitation energies, transition moments, and excited-state energy gradients on the nicotine molecule*, JOURNAL OF CHEMICAL PHYSICS **141**, 224114 (2014), DOI: [10.1063/1.4903307](https://doi.org/10.1063/1.4903307).

2013

- [13.01] V. Barone, M. Biczysko, J. Bloino, C. Puzzarini, *Glycine conformers: a never-ending story?* PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 1358-1363 (2013), DOI: 10.1039/c2cp43884d
- [13.02] G. Prampolini, F. Bellina, M. Biczysko, C. Cappelli, L. Carta, M. Lessi, A. Pucci, G. Ruggeri, V. Barone, *Computational design, synthesis, and mechanocromic properties of new thiophene-based π -conjugated chromophores*, CHEMISTRY **19**, 1996-2004 (2013), DOI: 10.1002/chem.201203672
- [13.03] A. Sgarbossa, S. Monti, F. Lenci, E. Bramanti, R. Bizzarri, V. Barone, *The effects of ferulic acid on β -amyloid fibrillar structures investigated through experimental and computational techniques*, BIOCHIMICA ET BIOPHYSICA ACTA **1830**, 2924–2937 (2013), DOI: 10.1016/j.bbagen.2012.12.023
- [13.04] V. Barone, C. Boilleau, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *Structure–Properties Relationships in Triplet Ground State Organic Diradicals: A Computational Study*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 300-307 (2013), DOI: 10.1021/ct300790c
- [13.05] V. Barone, M. Biczysko, J. Bloino, C. Puzzarini, *Characterization of the Elusive Conformers of Glycine from State-of-the-Art Structural, Thermodynamic, and Spectroscopic Computations: Theory Complements Experiment*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 1533-1547 (2013), DOI: 10.1021/ct3010672
- [13.06] F. Lipparini, F. Egidi, C. Cappelli, V. Barone, *The Optical Rotation of Methyloxirane in Aqueous Solution: A Never Ending Story?*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 1880-1884 (2013), DOI: 10.1021/ct400061z
- [13.07] V. Barone, C. Boilleau, I. Cacelli, A. Ferretti, G. Prampolini, *Conformational Effects on the Magnetic Properties of an Organic Diradical: A Computational Study*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 1958-1963 (2013), DOI: 10.1021/ct400020x
- [13.08] V. Barone, I. Carnimeo, G. Scalmani, *Computational Spectroscopy of Large Systems in Solution: The DFTB/PCM and TD-DFTB/PCM Approach*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 2052-2071 (2013), DOI: 10.1021/ct301050x
- [13.09] V. Barone, I. Cacelli, N. De Mitri, D. Licari, S. Monti, G. Prampolini, *JOYCE and ULYSSES: integrated and user-friendly tools for the parameterization of intramolecular force fields from quantum mechanical data*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 3736-3751 (2013), DOI: 10.1039/c3cp44179b.
- [13.10] M. Koenig, G. Bottari, G. Brancato, V. Barone, D. M. Guldi, T. Torres, *Unraveling the peculiar modus operandi of a new class of solvatochromic fluorescent molecular rotors by spectroscopic and quantum mechanical methods*, CHEMICAL SCIENCES **4**, 2502-2511 (2013), 10.1039/c3sc50290b
- [13.11] V. Barone, I. Cacelli, A. Ferretti, M. Vischiarelli, *Transport Properties of Binuclear Metal Complexes of the VIII Group Using a Simplified NEGF-DFT Approach*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **15**, 11409-11419 (2013), DOI: 10.1039/c3cp50974e
- [13.12] V. Barone, M. Biczysko, J. Bloino, C. Puzzarini, *Accurate Structure, Thermodynamic and*

Spectroscopic Parameters from CC and CC/DFT Schemes: the Challenge of the Conformational Equilibrium of Glycine, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 10094-10111 (2013), DOI: 10.1039/c3cp50439e

[13.13] V. Barone, M. Biczysko, J. Bloino, F. Egidi, C. Puzzarini, *Accurate Structure, Thermodynamics and Spectroscopy of Medium-Sized Radicals by Hybrid Coupled Cluster / Density Functional Theory Approaches: the Case of Phenyl Radical*, JOURNAL OF CHEMICAL PHYSICS **138**, 234303 (2013), DOI: 10.1063/1.4810863

[13.14] F. Lippalini, C. Cappelli, V. Barone, *A Gauge-Invariant Multiscale Approach to Magnetic Spectroscopies in Condensed Phase: General Three-Layer Model, Computational Implementation and Pilot Applications*, JOURNAL OF CHEMICAL PHYSICS **138**, 234108 (2013), DOI: 10.1063/1.4811113

[13.15] A. Pedone, E. Gambuzzi, V. Barone, S. Bonacchi, D. Genovese, E. Rampazzo, L. Prodi, M. Montalti, *Understanding the Photophysical Properties of Coumarin-Based Pluronic-Silica (Plus) Nanoparticles by means of Time-Resolved Emission Spectroscopy and Accurate TDDFT/Stochastic Calculations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 12360-12372 (2013), DOI: 10.1039/c3cp51943k

[13.16] S. Monti, E. Bramanti, V. Della Porta, M. Onor, A. D'Ulivo, V. Barone, *Interaction of Collagen with Chlorosulphurated Paraffin Tanning Agents: Fourier Transform Infrared Spectroscopic Analysis and Molecular Dynamics Simulations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 14736-14747 (2013), DOI: 10.1039/c3cp52404c

[13.17] I. Carnimeo, C. Puzzarini, N. Tasinato, P. Stoppa, A. Pietropolli Charmet, M. Biczysko, C. Cappelli, V. Barone, *Anharmonic Theoretical Simulations of Infrared Spectra of Halogenated Organic Compounds*, JOURNAL OF CHEMICAL PHYSICS, **139**, 074310 (2013), DOI: 10.1063/1.4817401

[13.18] A. Pezzella, O. Crescenzi, L. Panzella, A. Napolitano, E. J. Land, V. Barone, M. D'Ischia, *Free Radical Coupling of o-Semiquinones Uncovered*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **135**, 12142-12149 (2013), DOI: 10.1021/ja4067332

[13.19] G. Pescitelli, V. Barone, L. Di Bari, A. Rizzo, F. Santoro, *Vibronic Coupling Dominates the Electronic Circular Dichroism of the Benzene Chromophore (1)L_b Band*, JOURNAL OF ORGANIC CHEMISTRY **78**, 7398-7405 (2013), DOI: 10.1021/jo401112v

[13.20] M. Caricato, F. Lippalini, G. Scalmani, C. Cappelli, V. Barone, *Vertical Electronic Excitations in Solution with the EOM-CCSD Method Combined with a Polarizable Explicit / Implicit Solvent Model*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 3035-3042 (2013), DOI: 10.1021/ct4003288

[13.21] S. Monti, A. Corozzi, P. Fistrup, K. L. Yoshi, *Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 15062-15077 (2013), DOI: 10.1039/c3cp51931g

[13.22] C. Puzzarini, M. Biczysko, V. Barone, I. Peña, C. Cabezas, J. L. Alonso, *Accurate Molecular Structure and Spectroscopic Properties of Nucleobases: a Combined Computational-Microwave*

Investigation of 2-Thiouracil as a Case Study, PHYSICAL CHEMISTRY CHEMICAL PHYSICS
DOI: 10.1039/c3cp52347k (2013), DOI: 10.1039/c3cp52347k

[13.23] F. Egidi, J. Bloino, C. Cappelli, V. Barone, J. Tomasi, *Effective Tuning of NMR and EPR Parameters by Vibrational Averaging and Environmental Effects: an Integrated Computational Approach*, MOLECULAR PHYSICS **111**, 1345-1354 (2013), DOI: 10.1080/00268976.2013.796413

[13.24] Na Lin, V. Barone, C. Cappelli, X. Zhao, K. Ruud, F. Santoro, *Effective Time-Independent Studies on Resonance Raman Spectroscopy of Trans-Stilbene Including the Dushinsky Effect*, MOLECULAR PHYSICS **111**, 1511-1525 (2013), DOI: 10.1080/00268976.2013.809490

[13.25] M. Di Valentin, E. Salvadori, V. Barone, D. Carbonera, *Unravelling Electronic and Structural Requisites of Triplet-Triplet Energy Transfer by Advanced Electron Paramagnetic Resonance and Density Functional Theory*, MOLECULAR PHYSICS **111**, 2914-2932 (2013), DOI: 10.1080/00268976.2013.800602

[13.26] M. Zerbetto, D. Licari, V. Barone, A. Polimeno, *Computational Tools for the Interpretation of Electron Spin Resonance Spectra in Solution*, MOLECULAR PHYSICS **111**, 2746-2756 (2013); DOI: 10.1080/00268976.2013.800602

[13.27] F. Egidi, J. Bloino, C. Cappelli, V. Barone, *Development of a Virtual Spectrometer for Chiroptical Spectroscopies. The Case of Nicotine*, CHIRALITY **25**, 701-708 (2013), DOI: 10.1002/chir.22200

[13.28] S. Grubisic, G. Brancato, V. Barone, *An Improved Amber Force Field for alpha, alpha dialkylated peptides: intrinsic and Solvent-Induced Conformational Preferences of Model Systems*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 17395-17407 (2013), DOI: 10.1039/c3cp52721b

[13.29] A. Baiardi, J. Bloino, V. Barone, *General Time Dependent Approach to Vibronic Spectroscopy Including Franck-Condon, Herzberg-Teller, and Dushinsky Effects*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 4097-4115 (2013), DOI: 10.1021/ct400450k

[13.30] A. Pietropolli Charmet, P. Stoppa, N. Tasinato, S. Giorgianni, V. Barone, M. Biczysko, J. Bloino, C. Cappelli, I. Carnimeo, C. Puzzarini, *An integrated experimental and quantum-chemical investigation of the vibrational spectra of chlorofluoromethane*, JOURNAL OF CHEMICAL PHYSICS **139**, 164302 (2013), DOI: 10.1063/1.4825380

[13.31] N. De Mitri, S. Monti, G. Prampolini, V. Barone, *Absorption and Emission Spectra of a Flexible Dye in Solution: A Computational Time-Dependent Approach*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **9**, 4507-4516 (2013), DOI: 10.1021/ct4005799

[13.32] C. Merten, J. Bloino, V. Barone, Y. Xu, *Anharmonicity Effects in the Vibrational CD Spectra of Propylene Oxide*, JOURNAL OF PHYSICAL CHEMISTRY LETTERS **4**, 3424-3428 (2013), DOI: 10.1021/jz401854y

[13.33] L. Leone, O. Crescenzi, R. Amorati, L. Valgimigli, A. Napolitano, V. Barone, M. d'Ischia, *Red-hair inspired chromogenic system based on a proton-switched dehydrogenative free-radical coupling*, ORGANIC LETTERS **15**, 4944-4947 (2013), DOI: 10.1021/ol402161j

[13.34] C. Puzzarini, M. Biczysko, V. Barone, I. Pena, C. Cabezas, J.L. Alonso, *Accurate molecular structure and spectroscopic properties of nucleobases: a combined computational-microwave*

investigation of 2-thiouracil as a case study, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **15**, 16965-16975 (2013), DOI: 10.1039/c3cp52347k

[13.35] C. Zazza, G. Mancini, G. Brancato, V. Barone, *In silico study of molecular-engineered nanodevices: a lockable light-driven motor in dichloromethane solution*, JOURNAL OF PHYSICAL CHEMISTRY LETTERS, **4**, 3885-3890 (2013), DOI: 10.1021/jz4019404

[13.36] A. Maranzana, A. Giordana, A. Indarto, G. Tonachini, V. Barone, M. Causà, M. Pavone, *Density functional theory study of the interaction of vinyl radical, ethyne, and ethene with benzene, aimed to define an affordable computational level to investigate stability trends in large van der Waals complexes*, JOURNAL OF CHEMICAL PHYSICS **139**, 244306 (2013), DOI: 10.1063/1.4846295

[13.37] F.J. Avila Ferrer, V. Barone, C. Cappelli, F. Santoro, *Duschinsky, Herzberg-Teller, and Multiple Electronic Resonance Interferential Effects in Resonance Raman Spectra and Excitation Profiles. The Case of Pyrene*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 3597-3611 (2013), DOI: 10.1021/ct400197y.

[13.38] L. Hermosilla, G. Prampolini, P. Calle, J.M. Garcia de la Vega, G. Brancato, V. Barone, *Extension of the AMBER Force Field for Nitroxide Radicals and Combined QM/MM/PCM Approach to the Accurate Determination of EPR Parameters of DMPO-H in Solution*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **9**, 3626-3636 (2013), DOI: 10.1021/ct4003256

2012

- [12.01] V. Barone, M. Biczysko, J. Bloino, M. Borkowska-Panek, I. Carnimeo, P. Panek, *Toward anharmonic computations of vibrational spectra for large molecular systems*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **112**, 2185-2200 (2012).
- [12.02] C. Zazza, G. Mancini, G. Brancato, N. Sanna, V. Barone, *Neutral molecular shuttle in acetonitrile dilute solution: new insights from molecular dynamics and density functional theory*, COMPUTATIONAL AND THEORETICAL CHEMISTRY **985**, 53-61 (2012).
- [12.03] M. Biczysko, J. Bloino, I. Carnimeo, P. Panek, V. Barone, *Simulation of theoretical IR spectra for complex molecular systems from vibrational perturbative approaches: glycine as a test case*, JOURNAL OF MOLECULAR STRUCTURE **1009**, 74-82 (2012).
- [12.04] J. Bloino, M. Biczysko, V. Barone, *General perturbative approach for spectroscopy, thermodynamics and kinetics: methodological background and benchmark studies*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **8**, 1015-1036 (2012).
- [12.05] F. Egidi, J. Bloino, V. Barone, C. Cappelli, *Toward an accurate modeling of optical rotation for solvated systems: anharmonic vibrational contributions coupled to continuum solvation models*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **8**, 585-597 (2012).
- [12.06] C. Zazza, M. Rutigliano, N. Sanna, V. Barone, *Oxygen adsorption on beta-quartz model surfaces: insights from density functional theory computations and semiclassical time-dependent dynamics*, JOURNAL OF PHYSICAL CHEMISTRY A **116**, 1975-1983 (2012)
- [12.07] J. Bloino, V. Barone, *A second-order perturbation theory route to vibrational averages and transition properties of molecules: general formulation and application to infrared and vibrational circular dichroism spectroscopies*, JOURNAL OF CHEMICAL PHYSICS **136**, 124108 (2012)
- [12.08] S. Monti, A.C.T. van Duin, K. Sung-Yup, V. Barone, *Exploration of the conformational and reactive dynamics of glycine and diglycine on TiO₂: computational investigations in the gas phase and in solution*, JOURNAL OF PHYSICAL CHEMISTRY C **116**, 5141-5150 (2012).
- [12.09] M. Dargiewicz, M. Biczysko, R. Impronta, V. Barone, *Solvent effects on electron-driven proton-transfer processes: adenine-thymine base pairs*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 8981-8989 (2012).
- [12.10] C. Cappelli, J. Bloino, F. Lipparini, V. Barone, *Toward ab-initio anharmonic vibrational circular dichroism spectra in condensed phase*, JOURNAL OF PHYSICAL CHEMISTRY LETTERS **3**, 1766-1773 (2012).
- [12.11] A. Pedone, J. Bloino, V. Barone, *Role of host-guest interactions in tuning the optical properties of coumarin derivatives incorporated in MCM-41: a TD-DFT investigation*, JOURNAL OF PHYSICAL CHEMISTRY C **116**, 17807-17818 (2012).
- [12.12] L. Leone, O. Crescenzi, A. Napolitano, V. Barone, M. d'Ischia, *The Delta(2,2)'-Bi("H-1,4-benzothiazine) structural motif of red hair pigments revisited: photochromism and acidichromism in a unique four-state system*, EUROPEAN JOURNAL OF ORGANIC CHEMISTRY 5136-5140 (2012)

[12.13] E. Salvadori, M. Di Valentin, C. Kay, A. Pedone, V. Barone, D. Carbonera, *The electronic structure of the lutein triplet-state in plant light-harvesting complex II*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 12238-12251 (2012).

[12.14] V. Barone, A. Baiardi, M. Biczisko, J. Bloino, C. Cappelli, F. Lipparini, *Implementation and validation of a multi-purpose virtual spectrometer for large systems in complex environments*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 12404-12422 (2012).

[12.15] A. Weigel, M. Pfaffe, M. Sajadi, R. Mahrwald, R. Improta, V. Barone, D. Polli, G. Cerullo, N.P. Ernsting, F. Santoro, *Barrierless photoisomerization of the “simplest cyanine”: joining computational and femtosecond optical spectroscopies to trace the full reaction path*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 13350-13364 (2012).

[12.16] V. Barone, I. Cacelli, A. Ferretti, M. Visciarelli, *Theoretical study of a molecular junction with asymmetric current/voltage characteristics*, CHEMICAL PHYSICS LETTERS **549**, 1-5 (2012).

[12.17] S. Grubisic, G. Brancato, A. Pedone, V. Barone, *Extension of the AMBER force field to cyclic α,α -dialkylated peptides*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 15308-15320 (2012)

[12.18] F. Lipparini, C. Cappelli, V. Barone, *Linear response theory and electronic transition energies for a fully polarizable QM/classical Hamiltonian*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **8**, 4153-4165 (2012).

[12.19] F. Lipparini, C. Cappelli, G. Scalmani, N. De Mitri, V. Barone, *Analytical first and second derivatives for a fully polarizable QM/classical Hamiltonian*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION **8**, 4270-4278 (2012).

[12.20] M. J. Ablowitz, V. Barone, S. De Lillo, M. Sommacal, *Traveling waves in elastic rods with arbitrary curvature and torsion*, JOURNAL OF NONLINEAR SCIENCE **22**, 1013-1040 (2012).

[12.21] V. Barone, A. Ferretti, I. Pino, *Absorption spectra of natural pigments as sensitizers in solar cells by TD-DFT and MR-PT2: protonated cyanidin*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **14**, 16130-16137 (2012).

2011

[11-01] N. Rega, G. Brancato, A. Petrone, P. Caruso, V. Barone, *Vibrational analysis of XAFS thermal factors by ab-initio molecular dynamics. The Zn^{2+} aqueous solution as case study*, JOURNAL OF CHEMICAL PHYSICS, **134**, 074504 (2011).

[11-02] V. Barone, J. Bloino, S. Monti, A. Pedone, G. Prampolini, *Fluorescence spectra of organic dyes in solution: a time dependent multilevel approach*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 2160-2166 (2011).

[11.03] V. Barone, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *Singlet-triplet energy gap of a diarylnitroxide diradical by an accurate many-body perturbative approach*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 4709-4714 (2011).

[11-04] G. De Pretis, A. Cartoni, M. Rosi, V. Barone, C. Puzzarini, A. Troiani, *The proton affinity and gas-phase basicity of sulfur dioxide*, CHEMICAL PHYSICS PHYSICAL CHEMISTRY, **12**, 112-115 (2011).

- [11.05] V. Barone, S. De Lillo, G. Lupo, A. Polimeno, *Dirichlet to Neumann map for a nonlinear diffusion equation*, STUDIES IN APPLIED MATHEMATICS, **126**, 145-155 (2011).
- [11.06] D. Branduardi, M. De Vivo, N. Rega, V. Barone, A. Cavalli, *Methyl Phosphate Dianion Hydrolysis in Solution Characterized by Path Collective Variables Coupled with DFT-Based Enhanced Sampling Simulations*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 539-543 (2011).
- [11-07] V. Barone, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *An Integrated Protocol for the Accurate Calculation of Magnetic Interactions in Organic Magnets*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 699-706 (2011).
- [11-08] F. Trani, V. Barone, *Silicon Nanocrystal Functionalization: Analytic Fitting of DFTB Parameters*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 699-706 (2011).
- [11.09] V. Barone, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *Organic Functionalization and Optimal Coverage of a Silicon(111) Surface in Solvent: A Computational Study*, JOURNAL OF PHYSICAL CHEMISTRY C, **115**, 4145-4154 (2011).
- [11-10] S. Monti, G. Prampolini, V. Barone, *Interactions of Nucleotide Bases with Decorated Si Surfaces from Molecular Dynamics Simulations*, JOURNAL OF PHYSICAL CHEMISTRY C **115**, 9146-9156 (2011).
- [11.11] C. Puzzarini, V. Barone, *Extending the molecular size in accurate quantum-chemical calculations: The equilibrium structure and spectroscopic properties of uracil*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 7189-7197 (2011).
- [11.12] F. Santoro, C. Cappelli, V. Barone, *Effective Time-Independent Calculations of Vibrational Resonance Raman Spectra of Isolated and Solvated Molecules Including Duschinsky and Herzberg-Teller Effects*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 1824-1839 (2011).
- [11.13] E. Collini, S. Carlotto, C. Ferrante, R. Bozio, A. Polimeno, J. Bloino, V. Barone, E. Ronchi, L. Beverina and G. A. Pagani, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **13**, 12087-12094 (2011).
- [11.14] L. Capelli, O. Crescenzi, P. Manini, A. Pezzella, V. Barone, M. d'Ischia, *π -Electron Manipulation of the 5,6-Dihydroxyindole/Quinone System by 3-Alkynylation: Mild Acid-Mediated Entry to (Cross)-Conjugated Scaffolds and Paradigms for Medium-Tunable Chromophores*, JOURNAL OF ORGANIC CHEMISTRY, **76**, 4457-4466.
- [11.15] D. Dondi, P. Cimino, V. Barone, A. Buttafava, O. Lanzalunga, A. Faucitano, *Matrix EPR and QM Study of a Model Aromatic Thioether Radical-Cation*, TETRAHEDRON LETTERS **52**, 4097-4102 (2011).
- [11.16] A. Pedone, G. Prampolini, S. Monti, V. Barone, *Absorption and Emission of Fluorescent Silica Nanoparticles from TD-DFT/MM/PCM calculations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 16698-16697 (2011).
- [11.17] I. Carnimeo, M. Biczysko, J. Bloino, V. Barone, *Reliable Structural, Thermodynamic, and Spectroscopic Properties of Organic Molecules Adsorbed on Silicon Surfaces from Computational*

Modeling: the Case of Glycine@Si(100), PHYSICAL CHEMISTRY CHEMICAL PHYSICS **13**, 16713-16727 (2011).

[11.18] G. Pietraperzia, M. Pasquini, F. Mazzoni, G. Piani, M. Becucci, M. Biczysko, D. Michalski, J. Bloino, V. Barone, *Noncovalent Interactions in the Gas Phase: The Anisole–Phenol Complex*, JOURNAL OF PHYSICAL CHEMISTRY A, **115**, 9603-9611 (2011).

[11.19] C. Cappelli, F. Lipparini, J. Bloino, V. Barone, *Toward an Accurate Description of Anharmonic Infrared Spectra in Solution within the Polarizable Continuum Model: Reaction Field, Cavity Field and Nonequilibrium Effects*, JOURNAL OF CHEMICAL PHYSICS, **135**, 104505 (2011).

[11.20] F. Avila Ferrer, R. Improta, F. Santoro, V. Barone, *Estimating the Inhomogenous Broadening of Electronic Transitions in Solution by First-principle Quantum Mechanical Calculations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 17007-17012 (2011).

[11.21] S. Monti, I. Cacelli, A. Ferretti, G. Prampolini, V. Barone, *DNA complementary and partially complementary tethered to a functionalized substrate:a molecular dynamics approach to biosensing*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 12478-12487 (2011).

[11.22] A. Pedone, G. Prampolini, S. Monti, V. Barone, *Adsorption and emission spectra of fluorescent silica nanoparticles from TD-DFT/MM/PCM calculations*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 16689-16697 (2011).

[11.23] V. Barone, M. Casarin, D. Forrer, S. Monti, G. Prampolini, *Molecular Dynamics Simulations of the Self-Assembly of Tetraphenylporphyrin-Based Monolayers and Bilayers at a Silver Interface*, JOURNAL OF PHYSICAL CHEMISTRY C, **115**, 18434-18444 (2011).

[11.24] D. Picconi, V. Barone, A. Lami, V. F. Santoro, R. Improta, *The interplay between π/π^* and n/π^* excited states in gas-phase thymine: a quantum dynamical study*, CHEMPHYSCHM **12**, 1957-1968 (2011).

[11.25] F. Trani, G. Scalmani, G. Zheng, I. Carnimeo, M. Frisch, V. Barone, *Time Dependent Density Functional Tight Binding: New Formulation and Benchmark of Excited States*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 3304-3313 (2011).

[11.26] C. Puzzarini, M. Biczysko, V. Barone, *Accurate anharmonic vibrational frequencies for uracil: the performance of composite schemes and hybrid CC/DFT model*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 3702-3710 (2011).

[11.27] F. Lipparini, V. Barone, *Polarizable force fields and polarizable continuum model: a fluctuating charges/PCM approach. I: theory and implementation*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **7**, 3711-3724 (2011).

[11.28] G. Brancato, V. Barone, *Free energy landscapes of ion coordination in aqueous solution*, JOURNAL OF PHYSICAL CHEMISTRY B **115**, 12875–12878 (2011).

[11.29] A. Pedone, G. Prampolini, S. Monti, V. Barone, *Realistic Modeling of Fluorescent Dye-Doped Silica Nanoparticles: A Step Toward the Understanding of their Enhanced Photophysical Properties*, CHEMISTRY OF MATERIALS, **23**, 5016-5023 (2011).

[11.30] S. Monti, F. Cicogna, E. Passaglia, G. Prampolini, V. Barone, *Theoretical study of the*

conformational and optical properties of a fluorescent sensor grafted on apolar polymer structures, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **13**, 21471-21478 (2011).

[11.31] R. Improta, V. Barone, *Interplay between “Neutral” and “Charge-Transfer” Excimers Rules the Excited State Decay in Adenine-Rich Polynucleotides*, ANGEWANDTE CHEMIE INTERNATIONAL EDITION **50**, 12016-12019 (2011).

2010

[10-01] S. Carlotto, C. Ferrante, A. Polimeno, C. Benzi, V. Barone, *Interpretation of the emission fluorescence spectra of two fluoro-ionophores: DMABNCrown4 and DMABN-Crown5*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **110**, 368-375 (2010).

[10-02] F. Santoro, V. Barone, *Computational approach to the study of the line-shape of absorption and electronic circular dichroism spectra*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **110**, 476-486 (2010).

[10-03] R. Improta, A. Lami, V. Barone, F. Santoro, *Time dependent and time-independent approaches to the computation of absorption spectra in solution: uracil derivatives as a test case*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **110**, 624-636 (2010).

[10-04] C. Puzzarini, V. Barone, *Benchmark calculations for molecules in the gas phase: state-of-the-art coupled-cluster computations*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **110**, 637-655 (2010).

[10-05] A. Pedone, J. Bloino, S. Monti, G. Prampolini, V. Barone, *Absorption and Emission UV-Vis spectra of the TRITC fluorophore molecule in solution: a quantum mechanical study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 1000-1006 (2010).

[10-06] V. Barone, J. Bloino, M. Biczysko, *Validation of the DFT/N07D computational model on the magnetic, vibrational and electronic properties of vinyl radical*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 1092 – 1101 (2010).

[10-07] O. Taglialatela-Scafati, E. Fattorusso, A. Romano, F. Scala, V. Barone, P. Cimino, E. Stendardo, B. Catalanotti, M. Persico, C. Fattorusso, *Insights into the mechanism of action of plakortins, simple 1,2-dioxane antimalarials*, ORGANIC BIOMOLECULAR CHEMISTRY 846-856 (2010).

[10-08] M. Casarin, M. Di Marino, D. Forrer, M. Sambi, F. Sedona, E. Tondello, A. Vittadini, V. Barone, M. Pavone, *Coverage-dependent self-assembly patterns of iron phtalocyanine on Ag(110): a comprehensive STM/DFT study*, JOURNAL OF PHYSICAL CHEMISTRY C, **114**, 2144-2153 (2010).

[10.09] A. Pedone, V. Barone, *Unraveling Solvent Effects on the Electronic Absorption Spectra of TRITC Fluorophore in Solution: a Theoretical TD-DFT/PCM Study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 2722-2729 (2010).

- [10.10] C. Puzzarini, M. Biczysko, V. Barone, *Accurate harmonic/anharmonic vibrational frequencies for open-shell systems: performances of the B3LYP/N07D model for semirigid free radicals benchmarked by CCSD(T) computations*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **6**, 828-838 (2010).
- [10.11] V. Barone, M. Biczysko, P. Cimino, *Interplay of Stereoelectronic Vibrational and Environmental Effects in Tuning Physicochemical Properties of Carbon-Centered Radicals*, in Carbon-Centered Free Radicals and Radical Cations, M. D. E. Forbes Ed., John Wiley & Sons, 105 (2010).
- [10.12] V. Barone, M. Biczysko, G. Brancato, *Extending the Range of Computational Spectroscopy by QM/MM Approaches. Time-dependent and Time-independent routes. In Combining Quantum Mechanics and Molecular Mechanics, Some Recent Progresses in QM/MM*, J. Sabin, S. Canuto Eds. ADVANCES IN QUANTUM CHEMISTRY, Academic Press, **59**, 17 (2010).
- [10.13] P. Cimino, A. Pedone, E. Stendardo, V. Barone, *Interplay of stereo-electronic, environmental, and dynamical effects in determining the EPR parameters of aromatic spin-probes: INDCO as a test case*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 3741-3746 (2010).
- [10.14] V. Barone, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *Parameterization and validation of an accurate force-field for the simulation of alkyl-amine functionalized silicon (111) surfaces*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 4201-4209 (2010).
- [10.15] J. Bloino, M. Biczysko, F. Santoro, V. Barone, *General approach to compute vibrationally resolved one-photon electronic spectra*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **6**, 1256-1274 (2010).
- [10.16] F. Santoro, V. Barone, A. Lami, R. Improta, *The excited states of Adenine-Guanine stacked dimers in aqueous solution: a PCM/TD-DFT study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 4934-4948 (2010).
- [10.17] C. Cappelli, S. Monti, G. Scalmani, V. Barone, *On the Calculation of Vibrational Frequencies for Molecules in Solution Beyond the Harmonic Approximation*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **6**, 1660-1669 (2010).
- [10-18] G. de Petris, A. Cartoni, A. Troiani, V. Barone, P. Cimino, G. Angelini, O. Ursini, *Double C-H Activation of Ethane by Metal-free SO₂⁺ Radical Cations*, CHEMISTRY, **6**, 6234-6242 (2010).
- [10-19] A. Pedone, M. Biczysko, V. Barone, *Environmental Effects in Computational Spectroscopy: Accuracy and Interpretations*, CHEMICAL PHYSICAL CHEMISTRY, **11**, 1812-1832 (2010).
- [10-20] S. Monti, I. Cacelli, A. Ferretti, G. Prampolini, V. Barone, *Simulating DNA Hybridization on an Amine Functionalized Silicon Substrate*, JOURNAL OF PHYSICAL CHEMISTRY B, **114**, 8341-8349 (2010).
- [10-21] M. Biczysko, G. Scalmani, J. Bloino, V. Barone, *Harmonic and anharmonic vibrational frequency calculations with the double-hybrid B2PLYP method. Analytic second derivatives and benchmark studies*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **6**, 2115-2125 (2010).

- [10-22] M. Arzillo, A. Pezzella, O. Crescenzi, A. Napolitano, E. Land, V. Barone, M. D'Ischia, *Cyclic structural motifs in 5,6-dihydroxyindole polymerization uncovered: biomimetic modular build-up of a unique five-membered macrocycle*, ORGANIC LETTERS, **12**, 3250-3253 (2010).
- [10-23] V. Barone, J. Bloino, C. Guido, F. Lipparini, *A fully automated implementation of VPT2 infrared intensities*, CHEMICAL PHYSICS LETTERS, **496**, 157–161 (2010).
- [10-24] G. Brancato, N. Rega, V. Barone, *Uracil anion radical in aqueous solution: Thermodynamics versus Spectroscopy*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 10736-10739 (2010).
- [10-25] M. Pavone, M. Biczysko, N. Rega, V. Barone, *Magnetic properties of nitroxide spin-probes: reliable account of molecular motions and non specific solvent effects by time-dependent and time-independent approaches*, JOURNAL OF PHYSICAL CHEMISTRY B, **114**, 11509-11514 (2010).
- [10-26] V. Barone, J. Bloino, S. Monti, A. Pedone, G. Prampolini, *Theoretical multilevel approach for studying the photophysical properties of organic dyes in solution*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 10550-10561 (2010).
- [10-27] E. Stendardo, A. Pedone, P. Cimino, M. C. Menziani, O. Crescenzi, V. Barone, *Extension of the AMBER Force-Field for the Study of Large Nitroxides in Condensed Phases: An ab initio Parameterization*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **12**, 11697-11709 (2010).
- [10-28] S. Monti, I. Cacelli, A. Ferretti, G. Prampolini, V. Barone, *DNA Capture Mechanism on Silicon Nanowires: a Molecular Dynamics Approach*, MOLECULAR BIOSYSTEMS, **6**, 2230-2240 (2010).
- [10-29] N. Schiccheri, M. Pasquini, G. Piani, G. Pietraperzia, M. Becucci, M. Biczysko, V. Barone, *Integrated experimental and computational spectroscopy study on π-stacking interaction: the anisole dimer*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS 12, 13547-13554 (2010).
- [10.30] V. Barone, P. Cimino, A. Pedone, *An integrated computational protocol for the accurate prediction of EPR and PNMR parameters of nitroxide radicals in solution*, MAGNETIC RESONANCE IN CHEMISTRY, **48**, S11-S22 (2010).
- [10.31] I. Pino, M. Causà, V. Barone, *Bottom-up approach to innovative memory devices: II. Molecular adsorption on electrodes and the asymmetric response*, JOURNAL OF PHYSICAL CHEMISTRY C, **114**, 21439–21443 (2010).
- [10.32] G. Brancato, N. Rega, V. Barone, *Microsolvation of uracil anion radical in aqueous solution: a QM/MM study*, CHEMICAL PHYSICS LETTERS, **500**, 104-110 (2010).
- [10.33] C. Puzzarini, V. Barone, *Toward spectroscopic accuracy for open-shell systems: Molecular structure and hyperfine coupling constants of H₂CN, H₂CP, NH₂, and PH₂ as test cases*, JOURNAL OF CHEMICAL PHYSICS, **133**, 184301 (2010)

2009

- [9-01] M. Zerbetto, A. Polimeno, V. Barone, *Hydrodynamic modeling of diffusion tensor properties for flexible molecules*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **30**, 2-13 (2009).

- [09-02] C. Puzzarini, V. Barone, *The role of accurate quantum mechanical computations in the assignment of vibrational spectra for unstable free radicals: H₂CN and F₂CN as test cases*, CHEMICAL PHYSICS LETTERS, **467**, 276-280 (2009).
- [09-03] V. Barone, P. Cimino, *Validation of the B3LYP/N07D and PBE0/N07D computational models for the calculation of electronic g-tensors*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **5**, 192-199 (2009).
- [09-04] V. Barone, I. Cacelli, A. Ferretti, *Magnetizing coupling in bis-nitronyl-nitroxide radicals: the role of aromatic bridges*, JOURNAL OF CHEMICAL PHYSICS **130**, 094305 (2009).
- [09-05] V. Barone, M. Casarin, D. Forrer, M. Pavone, M. Sambi, A. Vittadini, *Role and effective treatment of dispersive forces in materials: polyethylene and graphite crystals as test cases*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **30**, 934-939 (2009).
- [09-06] V. Barone, J. Bloino, M. Biczysko, F. Santoro, *Fully integrated approach to compute vibrationally resolved optical spectra: from small molecules to macrosystems*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **5**, 540-554 (2009).
- [09-07] M. Biczysko, J. Bloino, V. Barone, *First principle simulation of vibrationally resolved A²B₁ ~X²A₁ electronic transition of phenyl radical*, CHEMICAL PHYSICS LETTERS, **471**, 143-147 (2009).
- [09-08] F. Trani, M. Causà, S. Lettieri, A. Setaro, D. Ninno, V. Barone, P. Maddalena, *Role of surface oxygen vacancies in photoluminescence of tin dioxide nanobelts*, MICROELECTRONICS JOURNAL, **40**, 236-238 (2009).
- [09-09] Na Lin, F. Santoro, A. Rizzo, Y. Luo, X. Zhao, V. Barone, *Vibrationally resolved two-photon circular dichroism spectra of (R)-(+)-3-methylcyclopentanone*, JOURNAL OF PHYSICAL CHEMISTRY A, **113**, 4198-4207 (2009).
- [09-10] A. Klamt, B. Mennucci, J. Tomasi, V. Barone, C. Curutchet, M. Orozco, F. J. Luque, *On the Performance of Continuum Solvation Methods. A Comment on “Universal Approaches to Solvation Modeling”*, ACCOUNTS OF CHEMICAL RESEARCH, **42**, 489-492 (2009).
- [09-11] N. Sanna, G. Chillemi, L. Gontrani, G. Mancini, S. Castelli, G. Zagotto, C. Zazza, V. Barone, A. Desideri, *UV-vis spectra of anticancer camptothecin drugs in aqueous solution: unraveling specific spectroscopic signatures by a combined computational and experimental study*, JOURNAL OF PHYSICAL CHEMISTRY B, **113**, 5369-5375 (2009).
- [09-12] M. Argeri, V. Barone, S. De Lillo, G. Lupo, M. Sommacal, *Elastic rods in life- and material-sciences. A general integrable model*, PHYSICA D, **238**, 1031-1049 (2009).
- [09-13] A. Pezzella, L. Panzella, O. Crescenzi, A. Napolitano, S. Navaratman, R. Edge, E. J. Land, V. Barone, M. D'Ischia, *Lack of Visible Chromophore Development in the Pulse Radiolysis/Oxidation of 5,6-dihydroxyndole-2-carboxylic Acid Oligomers: DFT Investigation and Implications for Eumelanin Absorption Properties*, JOURNAL OF ORGANIC CHEMISTRY, **74**, 3727-3734 (2009).

- [09-14] V. Barone, I. Cacelli, A. Ferretti, G. Prampolini, *Modified Virtual Orbitals for CI calculations of energy splitting in organic diradicals*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 3854-3860 (2009).
- [09-15] M. Biczysko, P. Panek, V. Barone, *Toward spectroscopic studies of biologically relevant systems: vibrational spectrum of adenine as a test case for performances of long-range/dispersion corrected density functional*, CHEMICAL PHYSICS LETTERS, **475**, 105-110 (2009).
- [09-16] M. Argeri, V. Barone, S. De Lillo, G. Lupo, M. Sommacal, *Existence of energy minima for elastic thin rods in static helical configurations*, THEORETICAL AND MATHEMATICAL PHYSICS, **159**, 698-711 (2009).
- [09-17] F. Santoro, R. Improta, V. Barone, *Three-Dimensional Diabatic Models for the $\pi\pi^*\rightarrow n\pi^*$ Excited-State Decay of Uracil Derivatives in Solution*, THEORETICAL CHEMISTRY ACCOUNTS, **123**, 273-286 (2009).
- [09-18] F. Williams, G. Chen, S. M. Mattar, P. H. Scudder, D. A. Trieber II, J. G. Saven, D. C. Whritenour, P. Cimino, V. Barone, *Magneto-structural relationships for radical cation and neutral pyridinophane structures with intrabridgehead nitrogen atoms. An integrated experimental and quantum mechanical study*, JOURNAL OF PHYSICAL CHEMISTRY B, **113**, 9026-9034 (2009).
- [09-19] R. Improta, C. Ferrante, R. Bozio, V. Barone, *The polarizability in solution of tetra-phenyl-porphyrin derivatives in their excited electronic states: a PCM/TD-DFT study*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 4664-4673 (2009).
- [09-20] R. Credendino, V. Barone, V. Busico, P.H.M.Buudzelaar, M.Causà, C.Zicovich-Wilson, *Periodic DFT-D modelling of bulk and surface properties of MgCl₂*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 6525-6532 (2009).
- [09-21] C. Puzzarini, V. Barone, *A theoretical study of the X₂NO systems (X=F,Cl,Br,I): effects of halogen substitution on structure, spectroscopy and energetic*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **5**, 2378-2387 (2009).
- [09-22] L. Dalla Via, S. Marciani Magno, O. Gia, A. M. Marini, F. Da Settimo, S. Salerno, C. La Motta, F. Simorini, S. Taliani, A. Lavecchia, C. Di Giovanni, G. Brancato, V. Barone, E. Novellino, *Benzothiopyranoindole-based antiproliferative agents: synthesis, cytotoxicity, nucleic acid interaction and topoisomerase inhibition properties*, JOURNAL OF MEDICINAL CHEMISTRY, **52**, 5429-5441 (2009).
- [09-23] R. Improta, V. Barone, *PCM/TD-DFT study of the two lowest excited states of uracil derivatives in solution: 3 The effect of the functional and of the cavity model*, THEOCHEM, **914**, 87-93 (2009).
- [09-24] R. Improta, V. Barone, A. Lami, F. Santoro, *Quantum Dynamics of the ultrafast $\pi\pi^*/n\pi^*$ population transfer in Uracil and 5Fluoro-Uracil in water and acetonitrile*, JOURNAL OF PHYSICAL CHEMISTRY B, **113**, 14491-14503 (2009).
- [09-25] F. Santoro, V. Barone, R. Improta, *The excited state decay of the A-T DNA: a PCM/DFT study in aqueous solution of the (9-methyl-adenine)₂-(1-methyl-thymine)₂ stacked tetramer*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **131**, 15232-15245 (2009).

- [09-26] M. Zerbetto, A. Polimeno, V. Barone, *Simulation of electron spin resonance spectroscopy in diverse environments: an integrated approach*, COMPUTER PHYSICS COMMUNICATIONS, **180**, 2680-2697 (2009).
- [09-27] G. Brancato, N. Rega, V. Barone, *Molecular dynamics simulations in a NpT ensemble using non-periodic boundary conditions*, CHEMICAL PHYSICS LETTERS, **483**, 177-181 (2009).
- [09-28] V. Barone, I. Cacelli, A. Ferretti, S. Monti, G. Prampolini, *Sensors for DNA Detection: Theoretical Investigation of the Conformational Properties of Immobilized Single-Strand DNA*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 10644 – 10656 (2009).
- [09-29] L. Sementa, M. D’Amore, V. Barone, V. Busico, M. Causà, *An ab-initio study of a, b, and γ crystal phases of TiCl₃: geometry, electronic structure, and magnetism*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 11264-11275 (2009).
- [09-30] C. Puzzarini, V. Barone, *On the Stability of X₂NO radicals (X=F,Cl,Br,I)*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **11**, 11463-11470 (2009).
- [09-31] V. Barone, I. Cacelli, A. Ferretti, G. Prampolini, *Accurate yet feasible post Hartree-Fock computation of magnetic interactions in large biradicals through a combined variational/perturbative approach: setup and validation*, JOURNAL OF CHEMICAL PHYSICS, **131**, 224103 (2009).
- [09-32] G. Pietraperzia, M. Pasquini, N. Schiccheri, G. Piani, M. Becucci, E. Castellucci, M. Biczysko, J. Bloino, V. Barone, *High Resolution Electronic Spectroscopy of the Anisole Dimer in a Molecular Beam: Equilibrium Structure of a Complex Stabilized by the Stacking Interaction*, JOURNAL OF PHYSICAL CHEMISTRY A, **113**, 14343-14351 (2009).
- [09-33] V. Barone, I. Cacelli, P. Cimino, A. Ferretti, S. Monti, G. Prampolini, *Magnetic interactions in phenyl-bridged nitroxide diradicals: conformational effects by multireference and broken symmetry DFT approaches*, JOURNAL OF PHYSICAL CHEMISTRY A, **113**, 15150-15155 (2009).
- [09-34] R. Impronta, F. Santoro, V. Barone, A. Lami, *Vibronic Model for the Quantum Dynamical Study of the Competition between Bright and Charge-Transfer Excited States in Single-Strand Polynucleotides: the Adenine Dimer Case*, JOURNAL OF PHYSICAL CHEMISTRY A, **113** 15346-15354 (2009).
- [09-35] M. Rutigliano, C. Zazza, N. Sanna, A. Pieretti, G. Mancini, V. Barone, M. Cacciatore, *Oxygen adsorption on b-cristobalite polymorph: ab-initio modeling and semiclassical time-dependent dynamics*, JOURNAL OF PHYSICAL CHEMISTRY A, **113**, 15366-15375 (2009).

2008

- [08-01] G. Brancato, N. Rega, V. Barone, *Microsolvation of the Zn(II) ion in aqueous solution: an hybrid QM/MM MD approach using non-periodic boundary conditions*, CHEMICAL PHYSICS LETTERS, **451**, 53-57 (2008).
- [08-02] M. Zerbetto, A. Polimeno, P. Cimino, V. Barone, *On the interpretation of cw-ESR spectra of tempo-palmitate in 5-cyanobiphenyl*, JOURNAL OF CHEMICAL PHYSICS, **128**, 024501 (2008).

- [08-03] V. Barone, M.Causà, *Structure and ESR features of a radiation-induced radical in α -glycine crystals*, CHEMICAL PHYSICS LETTERS, **452**, 89-93 (2008).
- [08-04] M. Pavone, N. Rega, V. Barone, *Implementation and validation of DFT-D for molecular vibrations and dynamics: the benzene dimer as a case study*, CHEMICAL PHYSICS LETTERS, **452**, 333-339 (2008).
- [08-05] G. Brancato, N. Rega, V. Barone, *A discrete/continuum QM/MM/MD study of the triplet state of acetone in aqueous solution*, CHEMICAL PHYSICS LETTERS, **454**, 202-206 (2008).
- [08-06] P. D'Angelo, V. Migliorati, G. Mancini, V. Barone, G. Chillemi, *Integrated experimental and theoretical approach for the structural characterization of Hg^{2+} aqueous solutions*, JOURNAL OF CHEMICAL PHYSICS **128**, 084502 (2008).
- [08-07] V. Barone, P. Cimino, *Accurate and feasible computations of structural and magnetic properties of large free radicals: the PBE0/N07D model*, CHEMICAL PHYSICS LETTERS, **454**, 139-143 (2008).
- [08-08] F. Santoro, V. Barone, R. Improta, *Can TD-DFT calculations accurately describe the excited states behavior of stacked nucleobases? The cytosine dimer as a test case*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **29**, 957-964 (2008).
- [08-09] G. Brancato, N. Rega, V. Barone, *Accurate TD-DFT calculations of near-edge x-ray and optical absorption spectra of liquid water using non-periodic boundary conditions: The role of self-interaction and long-range effects*, PHYSICAL REVIEW LETTERS, **100**, 107401 (2008).
- [08-10] G. Brancato, N. Rega, V. Barone, *A hybrid explicit/implicit solvation model for first principle molecular dynamics simulations in condensed phase*, JOURNAL OF CHEMICAL PHYSICS, **128**, 144501 (2008).
- [08-11] M. Di Valentin, S. Ceola, G. Agostini, G. M. Giacometti, A. Angerhofer, O. Crescenzi, V. Barone, D. Carbonera, *Pulse ENDOR and density functional theory on the peridinin triplet state involved in the photo-protective mechanism in the peridinin-chorophyll a-protein from amphidinium carterae*, BIOCHIMICA ET BIOPHYSICA ACTA (BBA) – BIOENERGETICS **1777**, 295-307 (2008).
- [08-12] G. Mancini, N. Sanna, V. Barone, P. D'Angelo, G. Chillemi, *Structural and dynamical properties of the Hg^{2+} aqua ion: a Molecular Dynamics study*, JOURNAL OF PHYSICAL CHEMISTRY B, **112**, 4694-4702 (2008).
- [08-13] V. Barone, M. Biczysko, M. Pavone, *The role of dispersion correction to DFT for modeling weakly bound molecular complexes in the ground and excited electronic states*, CHEMICAL PHYSICS, **347**, 247-256 (2008).
- [08-14] M. D'Ischia, O. Crescenzi, A. Pezzella, M. Arzillo, L. Panzella, A. Napolitano, V. Barone, *Structural effects on the electronic absorption properties of 5,6-dihydroxyindole oligomers: the potential of an integrated experimental and DFT approach to model eumelanin optical properties*, PHOTOCHEMISTRY AND PHOTOBIOLOGY, **84**, 600-607 (2008).
- [08-15] V. Barone, I. Cacelli, A. Ferretti, M. Girlanda, *Toward an effective yet reliable many-body computation of magnetic couplings in bis-nitronyl nitroxide biradicals*, JOURNAL OF CHEMICAL PHYSICS, **128**, 174303 (2008).

- [08-16] V. Barone, P. Cimino, E. Stendardo, *Development and validation of the B3LYP/N07D computational model for structural parameter and magnetic tensors of large free radicals*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **4**, 751-764 (2008).
- [08-17] V. Barone, R. Improta, N. Rega, *Quantum mechanical computations and spectroscopy: from small rigid molecule in the gas phase to large flexible molecule in solution*, ACCOUNTS OF CHEMICAL RESEARCH, **41**, 605-616 (2008).
- [08-18] F. Trani, M. Causà, D. Ninno, G. Canale, V. Barone, *Density functional study of the SnO₂ surface and subsurface sites*, PHYSICAL REVIEW B, **77**, 245410 (2008).
- [08-19] G. Brancato, N. Rega, M. Causà, V. Barone, *Theoretical modeling of open-shell molecules in solution: a QM/MM molecular dynamics approach*, THEORETICAL CHEMISTRY ACCOUNTS, **120**, 499-506 (2008).
- [08-20] R. Improta, V. Barone, *The excited states of adenine and thymine nucleoside and nucleotide in aq ueous solution: a comparative study by Time-Dependent DFT calculations*, THEORETICAL CHEMISTRY ACCOUNTS, **120**, 491-497 (2008).
- [08-21] F. Santoro, A. Lami, R. Improta, J. Bloino, V. Barone, *Effective method for the computation of optical spectra of large molecules at finite temperature including the Duschinsky and Herzberg-Teller effect. The Q_x band of porphyrin as a case study*, JOURNAL OF CHEMICAL PHYSICS, **128**, 224311 (2008).
- [08-22] J. Bloino, M. Biczysko, O. Crescenzi, V. Barone, *Integrated computational approach to vibrationally resolved electronic spectra: anisole as a test case*, JOURNAL OF CHEMICAL PHYSICS, **128**, 244105 (2008).
- [08-23] S. Carlotto, A. Polimeno, C. Ferrante, C. Benzi, V. Barone, *An integrated approach for modeling the fluorescence of DMABN in polar environments*, JOURNAL OF PHYSICAL CHEMISTRY B, **112**, 8106-8113 (2008).
- [08-24] V. Barone, G. Brancato, R. Improta, *Toward an integrated computational approach for the description of localized physico-chemical properties involving biomolecules*, in Computational Proteomics, M.Gomez, Ed., Transworts Research (2008) pp. 1-24.
- [08-25] C. Puzzarini, V. Barone, *A critical analysis of the structure and vibrational frequencies of F₂NO⁺ and Cl₂NO⁺ from accurate quantum chemical computations*, CHEMICAL PHYSICS LETTERS, **462**, 49-52 (2008).
- [08-26] C. Puzzarini, V. Barone, *Toward spectroscopic accuracy for organic free radicals: molecular structure, vibrational spectrum and magnetic properties of F₂NO*, JOURNAL OF CHEMICAL PHYSICS, **129**, 084306 (2008).
- [08-27] V. Labet, C. Morell, A. Grand, J. Cadet, P. Cimino, V. Barone, *Cross-linked adducts between guanine and thymine mediated by hydroxyl radical and one-electron oxidation: a theoretical study*, ORGANIC BIOMOLECULAR CHEMISTRY, **6**, 3300-3305 (2008).
- [08-28] B. Pagano, M. Pavone, A. L.Piccinelli, L. Rastrelli, O. Cuesta-Rubio, V. Barone, C. A. Mattia, *Structural and conformational investigation of nemorosone: a combined X ray and ab initio study*, CHEMICAL PHYSICS LETTERS, **462**, 158-163 (2008).

- [08-29] M. Della Greca, M. R. Iesce, L. Previtera, M. Rubino, V. Barone, O. Crescenzi, *Phototransformation of the drug trazodone in aqueous solution*, JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY A: CHEMISTRY, **199**, 353-357 (2008).
- [08-30] P. Manini, L. Capelli, M. Arzillo, O. Crescenzi, A. Napolitano, V. Barone, M. d'Ischia, *Chemistry of nitrated lipids: remarkable instability of 9-nitrolinoleic acid in neutral aqueous medium and a novel nitronitrate ester product by concurrent autoxidation/nitric oxide-release pathways*, JOURNAL OF ORGANIC CHEMISTRY, **73**, 7517-7525 (2008).
- [08-31] F. De Angelis, F. Santoro, M. K. Nazeruddin, V. Barone, *Ab-initio prediction of the emission color in Phosphorescent Iridium (III)- complexes for OLEDs*, JOURNAL OF PHYSICAL CHEMISTRY B, **112**, 13181-13183 (2008).
- [08-32] C. Puzzarini, V. Barone, *Assessment of a computational strategy approaching spectroscopic accuracy for structure, magnetic properties and vibrational frequencies of organic free radicals: the F_2CN and F_2BO case*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **10**, 6991-6997 (2008).
- [08-33] I. Pino, M. Causà, V. Barone, *Bottom-up approach to innovative memory devices. I. Intrinsic and environmental effects on the molecular component*, JOURNAL OF PHYSICAL CHEMISTRY C, **112**, 17081-17088 (2008).
- [08-34] F. Santoro, V. Barone, R. Improta, *First principle calculations shed new light on the excited state behaviour of T-A DNA*, CHEMPHYSCHM, **9**, 2531-2537 (2008).
- [08-35] S. Carlotto, C. Benzi, R. Riccò, C. Ferrante, M. Magini, A. Polimeno, V. Barone, *An integrated approach for the interpretation of emission fluorescence of DMABN-Crown derivatives in polar environments*, CHEMICAL PHYSICS LETTERS, **467**, 204-209 (2008).
- [08-36] N. Lin, F. Santoro, X. Zhao, A. Rizzo, V. Barone, *Vibronically resolved electronic circular dichroism spectra of R-(+)-3-methyl-cyclopentanone: a theoretical study*, JOURNAL OF PHYSICAL CHEMISTRY B, **112**, 12401-12411 (2008).
- [08-37] M. Causà, V. Barone, M. Stener, G. Fronzoni, *Electrostatic effects on cluster simulation of ionic crystals and surfaces*, JOURNAL OF PHYSICS CONFERENCE SERIES **117**, 012009 (2008).
- [08-38] S. Lettieri, M. Causà, A. Setaro, F. Trani, V. Barone, D. Ninno, P. Maddalena, *Direct role of surface oxygen vacancies in visible light emission of tin dioxide nanowires*, JOURNAL OF CHEMICAL PHYSICS, JOURNAL OF CHEMICAL PHYSICS **129**, 244710 (2008).
- [08-39] A. Pedone, M. Pavone, C. Menziani, V. Barone, *Accurate First-Principle Prediction of ^{29}Si and ^{17}O NMR Parameters in SiO_2 polymorphs: The cases of zeolites Sigma-2 and Ferrierite*, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, **4**, 2130-2140 (2008).
- [08-40] M. Causà, M. Pavone, F. Trani, V. Barone, *Computational materials science at work: density functional based study of structural and optical properties of Tin Oxide surfaces*, NUOVO CIMENTO B **123**, 1381-1390 (2008).

- [07-01] R. Improta, V. Barone, F. Santoro, *Ab-initio computation of absorption spectra of large molecules in solution*, ANGEWANDTE CHEMIE, **46**, 405-408 (2007).
- [07-02] F. Pepi, A. Ricci, V. Barone, P. Cimino, *Gas phase ion chemistry of diphosphate anions as a tool to investigate the intrinsic requirements of phosphate esters enzymatic reactions. The $[M^I M^{II} HP_2O_7]^-$ ions*, CHEMISTRY, **13**, 2096-2108 (2007).
- [07-03] F. Santoro, R. Improta, A. Lami, J. Bloino, V. Barone, *An effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution*, JOURNAL OF CHEMICAL PHYSICS, **126**, 084509 (2007).
- [07-04] A. Pezzella, A. Natangelo, L. Panzella O. Crescenzi, A. Napolitano, S. Navaratman, R. Edge, E.J. Land, V. Barone, M. d'Ischia, *A Novel Labile 5,6-Indolequinone and Transient Semiquinone Precursor by Oxidation of 5,6-Dihydroxy-3-iodoindole*, JOURNAL OF ORGANIC CHEMISTRY, **72**, 1595-1603 (2007).
- [07-05] M. Zerbetto, S. Carlotto, A. Polimeno, C. Corvaja, L. Franco, C. Toniolo, F. Formaggio, V. Barone, P. Cimino, *Ab-Initio Modeling of CW-ESR Spectra of the Double Spin Labeled Peptide Fmoc-(Aib-Aib-TOAC)₂-Aib-OMe in Acetonitrile*, JOURNAL OF PHYSICAL CHEMISTRY B, **111**, 2868-2874 (2007).
- [07-06] G. Chillemi, G. Mancini, N. Sanna, V. Barone, S. Della Longa, M. Benfatto, N. V. Pavel, P. D'Angelo, *Evidence for seven-fold coordination in the first solvation shell of Hg(II) aqua ion from a combined experimental/computational approach*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **129**, 5430-5436 (2007).
- [07-07] V. Barone, *Theoretical and computational chemistry in Italy: an overview*, THEORETICAL CHEMISTRY ACCOUNTS, **117**, 599-602 (2007).
- [07-08] G. Brancato, N. Rega, V. Barone, *Theoretical modeling of spectroscopic properties of molecules in solution: toward an effective dynamical discrete/continuum approach*, THEORETICAL CHEMISTRY ACCOUNTS, **117**, 1001-10015 (2007).
- [07-09] R. Improta, V. Barone, F. Santoro, *Excited states properties of large molecules in solution: from structure to reactivity*, THEORETICAL CHEMISTRY ACCOUNTS, **117**, 1073-1084 (2007).
- [07-10] N. Sanna, T. Castrignano, P. D'Onorio De Meo, D. Carrabino, A. Grandi, G. Morelli, P. Caruso, V. Barone, *Gaussian Grid: a computational chemistry experiment over a web service oriented grid*, THEORETICAL CHEMISTRY ACCOUNTS, **117**, 1145-1152 (2007).
- [07-11] F. Santoro, R. Improta, A. Lami, V. Barone, *An effective method to compute Franck-Condon integrals for optical spectra of large molecules in solution. II: inclusion of thermal effects*, JOURNAL OF CHEMICAL PHYSICS, **126**, 184102 (2007).
- [07-12] V. Barone, P. Cimino, O. Crescenzi, M. Pavone, *Ab initio computation of spectroscopic parameters as a tool for the structural elucidation of organic systems*, THEOCHEM, **811**, 323-335 (2007).
- [07-13] F. Santoro, V. Barone, R. Improta, *Understanding the influence of base stacking on excited-state dynamics in DNA: a TD-DFT study of 9-methyl adenine oligomers in aqueous solution*, PNAS, **104**, 9931-9936 (2007).

[07-14] V. Barone, R. Improta, G. Morelli, F. Santoro, *UV-vis spectra of p-benzoquinone radical anion by a TD-DFT/PCM approach*, THEORETICAL CHEMISTRY ACCOUNTS, **118**, 143-148 (2007).

[07-15] I. Borriello, G. Cantele, D. Ninno, G. Iadonisi, M. Cossi, V. Barone, *Ab-initio study of electron affinity variation induced by organic molecules adsorption on the silicon (001) surface*, PHYSICAL REVIEW B **76**, 035430 (2007).

[07-16] M. Pavone, P. Cimino, O. Crescenzi, A. Sillnppää, V. Barone, *Interplay of intrinsic, environmental, and dynamic effects in tuning the EPR parameters of nitroxides: further insights from an integrated computational approach*, JOURNAL OF PHYSICAL CHEMISTRY B **111**, 8928-8939 (2007).

[07-17] R. Improta, G. Scalmani, M. J. Frisch, V. Barone, *A rigorous and accurate method for computing fluorescence energies in solution by means of State-Specific PCM TD-DFT calculations*, JOURNAL OF CHEMICAL PHYSICS **127**, 074504 (2007).

[07-18] P. Cimino, M. Pavone, V. Barone, *Halogen bonds between TEMPO radical and $C_xH_yF_zI$ species: DFT calculations of physico-chemical properties and comparison with hydrogen bonded adducts*, JOURNAL OF PHYSICAL CHEMISTRY A **111**, 8482-8490 (2007).

[07-19] S. Carlotto, P. Cimino, M. Zerbetto, L. Franco, C. Corvaja, M. Crisma, F. Formaggio, C. Toniolo, A. Polimeno, V. Barone, *Unraveling solvent driven equilibria between α - and 310-helices through an integrated spin labelling and computational approach*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **129**, 11248-11258 (2007).

[07-20] I. S. Lim, P. Botschwina, R. Oswald, V. Barone, H. Stoll, P. Schwerdtfeger, *Calculated spectroscopic and electric properties of the alkali metal-ammonia complexes from $Kn-NH_3$ to Fr_n-NH_3 ($n = 0, +1$)*, JOURNAL OF CHEMICAL PHYSICS **127**, 104313 (2007).

[07-21] V. Barone, A. Polimeno, *From vertical excitation energies of isolated molecules to complete UV/vis spectra of flexible molecules in solution*, CHEMICAL SOCIETY REVIEWS, **36**, 1724-1731 (2007).

[07-22] M. Biczysko, G. Piani, M. Pasquini, N. Schiccheri, G. Pietrapiezzi, M. Becucci, M. Pavone, V. Barone, *On the properties of microsolvated molecule in the ground (S_0) and excited (S_1) states: the anisole-ammonia 1:1 complex*, JOURNAL OF CHEMICAL PHYSICS **127**, 144303 (2007).

[07-23] G. Brancato, N. Rega, V. Barone, *Unraveling the role of stereo-electronic, dynamical, and environmental effects in tuning the structure and magnetic properties of glycine radical in aqueous solution at different pH values*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **129**, 15380-15390 (2007).

[07-24] G. Piani, M. Pasquini, N. Schiccheri, G. Pietrapiezzi, M. Becucci, M. Biczysko, M. Pavone, V. Barone, *Olisotopomeric conformational changes in the anisole-water complex: new insights from HR-UV spectroscopy and theoretical studies*, JOURNAL OF PHYSICAL CHEMISTRY A **111**, 12363-12371 (2007).

[07-25] M. De Lucia, F. Mainieri, L. Verotta, M. Maffei, L. Panzella, O. Crescenzi, A. Napolitano, V. Barone, G. Appendino, M. D'Ischia, *Nitration vs. nitrosation chemistry of menthofuran: remarkable fragmentation and dimerization pathways and expeditious entry into dehydromenthofurolactone*, JOURNAL OF ORGANIC CHEMISTRY **72**, 10123-10129 (2007).

[07-26] R. Improta, V. Barone, F. Santoro, *Accurate steady state and zero-time fluorescence spectra of large molecules in solution by a first principle computational method*, JOURNAL OF PHYSICAL CHEMISTRY B **111**, 14080-14082 (2007).

[07-27] V. Barone, P. Cimino, M. Pavone, *EPR spectra of organic free radicals in solution from an integrated computational approach* in B.Mennucci, R. Cammi Eds. Continuum Solvation Models in Chemical Physics. From Theory to Applications, John Wiley & Sons (2007) pp.145-166.

2006

[06-01] V.Barone, F.De Rienzo, E.Langella, M.C.Menziani, N.Regia, M.Sola, *A computational protocol to probe the role of solvation effects on the reduction potential of azurine mutants*, PROTEINS **62**, 262-269 (2006).

[06-02] P.Cimino, M.Pavone, V.Barone, *Structural, Thermodynamic, and Magnetic Properties of Adducts between TEMPO Radical and Alcohols in Solution: New Insights from DFT and Discrete-Continuum Solvent Models*, CHEMICAL PHYSICS LETTERS **409**, 106-110 (2006).

[06-03] M.Pavone, G.Brancato, G.Morelli, V.Barone, *Spectroscopic properties in liquid phase: combining ab-initio calculations and classical molecular dynamics*, CHEMPHYSCHM **7**, 148-156 (2006).

[06-04] T.Gustavsson, A.Banyasz, E.Lazzarotto, D.Markovitsi, G.Scalmani, M.Frisch, R.Improta, V.Barone, *Understanding the excited state behavior of uracil and thymine: an integrated experimental and computational study of 11 uracil derivatives in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 607-619 (2006).

[06-05] M.D'Amore, G.Talarico, V.Barone, *Periodic and high temperature disordered conformations of polytetrafluoroethylene chains: an ab-initio modelling*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 1099-1108 (2006).

[06-06] G.Cantele, F.Trani, D.Ninno, M.Cossi, V.Barone, *A theoretical study of ethylene, cyclopentene and 1-amino-3-cyclopentene adsorption on the silicon <100> surface*, JOURNAL OF PHYSICS: CONDENSED MATTER **18**, 2349-2365 (2006).

[06-07] M.Pavone, P.Cimino, F.De Angelis, V.Barone, *Interplay of stereo-electronic and enviromental effects in tuning the structural and magnetic properties of a prototypical spin probe: insights from a first principle dynamical approach*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 4338-4347 (2006).

[06-08] P.Cimino, R.Improta, G.Bifulco, R.Riccio, L.Gomez-Paloma, V.Barone, *Alkylation properties of duocarmycins: DFT studies suggest new crucial factors determining reactivity*, ORGANIC BIOLOGICAL CHEMISTRY **4**, 1242-1251 (2006).

[06-09] G.Scalmani, M.J.Frisch, B.Mennucci, J.Tomasi, R.Cammi, V.Barone, *Geometries and Properties of Excited states in the Gas Phase and in Solution. Theory and Application of a Time-Dependent DFT Polarizable Continuum Model*, JOURNAL OF CHEMICAL PHYSICS **124**, 094107 (2006).

- [06-10] C.Adamo, V.Barone, A.Bencini, R.Broer, M.Filatov, N.M.Harrison, F.Illas, J.P.Malrieu, P.R.Moreira, Comment on “*About the Calculation of Exchange Coupling Constants Using Density-Functional Theory: the Role of the Self-interaction Error*”, JOURNAL OF CHEMICAL PHYSICS **124**, 107101 (2006).
- [06-11] M.De Lucia, L.Panzella, O.Crescenzi, A.Napolitano, V.Barone, M.d’Ischia, *The catecholic antioxidant piceatannol is an effective nitrosation inhibitor via an unusual double bond nitration*, BIOORGANIC & MEDICINAL CHEMISTRY LETTERS **16**, 2238-2242 (2006).
- [06-12] N.Regia, G.Brancato, V.Barone, *Ab-initio molecular dynamics in condensed phase using localized basis functions and non periodic boundary conditions*, CHEMICAL PHYSICS LETTERS **422**, 367-371 (2006).
- [06-13] I.Ciofini, L.Joubert, M.Pavone, V.Barone, C.Adamo, *Theoretical insights on the chemical reactivity of metallo-porphyrins using density functional theory*, in N₄-Macrocyclic metal complexes, J. Zagal, F. Bedioui, J.P. Dodelet eds., Springer (Berlin) (2006).
- [06-14] M.F.Iozzi, M.Cossi, R.Improta, N.Regia, V.Barone, *A generalized polarizable continuum model for the study of heterogeneous dielectric environments*, JOURNAL OF CHEMICAL PHYSICS **124**, 184103 (2006).
- [06-15] E.Langella, R.Improta, O.Crescenzi, V.Barone, *Assessing the acid-base and conformational properties of histidine residues in human prion protein (125-228) by means of pKa calculations and molecular dynamics simulations*, PROTEINS **64**, 167-177 (2006).
- [06-16] R.Improta, V.Barone, M.D.Newton, *A parameter free quantum mechanical approach to the calculation of electron transfer rates for large systems in solution*, CHEMPHYSCHM **7**, 1211-1219 (2006).
- [06-17] G.Brancato, N.Regia, V.Barone, *Reliable molecular simulations of solute-solvent systems with a minimum number of solvent shells*, JOURNAL OF CHEMICAL PHYSICS **124**, 214505 (2006).
- [06-18] V.Barone, M.D.Newton, R.Improta, *New hints about dissociative electron transfer in D-peptide-A models from a density functional / polarizable continuum model*, JOURNAL OF PHYSICAL CHEMISTRY B **110**, 12632-12639 (2006).
- [06-19] T. Gustavsson, N. Sarkar, E. Lazzarotto, D. Markovitsi, V. Barone, R. Improta, *Solvent effect on the singlet excited state dynamics of 5-fluorouracyl in acetonitrile as compared to water*, JOURNAL OF PHYSICS B **110**, 12843-12847 (2006).
- [06-20] R. Improta, V. Barone, G. Scalmani, M.J. Frisch, *A State-Specific PCM TD-DFT method for equilibrium and non equilibrium excited state calculations in solution*, JOURNAL OF CHEMICAL PHYSICS **125**, 054103 (2006).
- [06-21] G. Rauhut, V. Barone, P. Schwerdtfeger, *Vibrational analysis for CHFClBr and CDFClBr based on high level ab-initio calculations*, JOURNAL OF CHEMICAL PHYSICS **125**, 054308 (2006).

- [06-22] M. Pavone, A. Sillampa, P. Cimino, O. Crescenzi, V. Barone, *Evidence of variable H-bonding networks embedding nitroxide free-radicals in protic solvents*, JOURNAL OF PHYSICAL CHEMISTRY B **110**, 16189-16192 (2006).
- [06-23] M. Pavone, O. Crescenzi, G. Morelli, N. Rega, V. Barone, *Solvent effects on the UV ($n \rightarrow \pi^*$) and NMR (^{17}O) spectra of acetone in aqueous solution. Development and validation of a modified AMBER force field for an integrated MD/DFT/PCM approach*, THEORETICAL CHEMISTRY ACCOUNTS **116**, 456-461 (2006).
- [06-24] L. Joubert, M. Pavone, V. Barone, C. Adamo, *A comparative static and dynamic study of a prototype SN2 reaction*, JOURNAL OF COMPUTATIONAL AND THEORETICAL CHEMISTRY **2**, 1220-1227 (2006).
- [06-25] V. Barone, A. Polimeno, *Integrated computational approaches to modelling of ESR observables*, PHYSCHEMCHEMPHYS **8**, 4609-4629 (2006).
- [06-26] B. Xerri, C. Morell, A. Grand, J. Cadet, P. Cimino, V. Barone, *Radiation induced formation of DNA intrastrand crosslinks between thymine and adenine bases: a theoretical approach*, ORGANIC BIOMOLECULAR CHEMISTRY **4**, 3986-3992 (2006).
- [06-27] M. Rutigliano, A. Pieretti, M. Cacciatore, N. Sanna, V. Barone, *N atoms recombination on a silica surface: a global theoretical approach*, SURFACE SCIENCE **600**, 4239-4246 (2006).
- [06-28] G. Brancato, N. Rega, V. Barone, *A QM/MM/MF molecular dynamics study of acrolein in aqueous solution: analysis of H-bonding and bulk effects on spectroscopic properties*, JOURNAL OF CHEMICAL PHYSICS **125**, 164515 (2006).
- [06-29] C. Benzi, M. Cossi, V. Barone, R. Tarroni, C. Zannoni, *Order Parameters of α, ω -diphenylpolyenes in a nematic Liquid Crystal from an Integrated Computational and ^{13}C NMR Spectroscopic Approach*, JOURNAL OF CHEMICAL PHYSICS **125**, 174904 (2006).
- [06-30] A. Pezzella, L. Panzella, O. Crescenzi, A. Napolitano, S. Navaratman, R. Edge, E.J. Land, V. Barone, M. d'Ischia, *Short-lived Quinonoid Species From 5,6-Dihydroxyindole Dimers en route to Eumelanin Polymers: First Investigation by an Integrated Chemical, Pulse Radiolytic and Quantum Mechanical Approach*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 15490-15498 (2006).
- [06-31] V. Barone, M. Brustolon, P. Cimino, A. Polimero, M. Zerbetto, A. Zoleo, *Development and validation of an integrated computational approach for the modeling of cw-ESR spectra of free radicals in solution. P-(methyl-thio)phenyl-nitronyl-nitroxide in toluene as a case study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 15865-15873 (2006).
- [06-32] F. Santoro, V. Barone, T. Gustavsson, R. Impronta, *Solvent effect on the singlet excited-state lifetimes of nucleic acid bases: a computational study of 5-fluorouracil and uracil in acetonitrile and water*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **128**, 16312-16322 (2006).

2005

- [05-01] V. Barone, *Anharmonic vibrational properties by a fully automated second order perturbative approach*, JOURNAL OF CHEMICAL PHYSICS **122**, 014108 (2005).

- [05-02] O.Crescenzi, M.Pavone, F.de Angelis, V.Barone, *Solvent effects on the UV($n \rightarrow \pi^*$) and NMR (^{13}C and ^{17}O) spectra of acetone in aqueous solution. An integrated Car Parrinello and DFT/PCM approach*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 445-453 (2005).
- [05-03] R.Improta, S.Antonello, F.Formaggio, F.Maran, N.Regia, V.Barone, *Understanding electron transfer across negatively-charged Aib oligo-peptides*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 1023-1033 (2005).
- [05-04] P.Carbonniere, T.Lucca, C.Pouchan, N.Regia, V.Barone, *Vibrational computations beyond the harmonic approximation: performances of the B3LYP functional for semirigid molecules*, JOURNAL OF COMPUTATIONAL CHEMISTRY **26**, 384-388 (2005).
- [05-05] I.Ciofini, C.Adamo, V.Barone, G.Berthier, A.Rassat, *Mapping the many electron generalised spin-exchange Hamiltonian to accurate post-HF calculations*, CHEMICAL PHYSICS **309**, 133-141 (2005).
- [05-06] C.Benzi, M.Cossi, V.Barone, R.Tarroni, C.Zannoni, *A combined theoretical and experimental approach to determining order parameters of solutes in liquid crystals from ^{13}C NMR data*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 2584-2590 (2005).
- [05-07] A.Pezzella, P.Manini, A.Napolitano, O.Crescenzi, V.Barone, M.d'Ischia, *Oxidative chemistry of 2- and 4-nitroestradiol: remarkable control of nitro group conformation over evolution of phenoxy radicals and novel potential routes for oxyfunctionalization of steroid scaffolds*, STEROIDS **70**, 543-550 (2005).
- [05-08] P.Cimino, V.Barone, *Solvent effects on molecular interactions: new hints from and integrated density functional / polarizable continuum model*, THEOCHEM **729**, 1-9 (2005).
- [05-09] G.Brancato, A. Di Nola, V.Barone, A.Amadei, *A mean field approach for molecular simulations of fluid systems*, JOURNAL OF CHEMICAL PHYSICS **122**, 154109 (2005).
- [05-10] G.Festa, M.Cossi, V.Barone, G.Cantele, D.Ninno, G.Iadonisi, *A first-principle study of the adsorption of 1-amino-3-cyclopentene on the (100) silicon surface*, JOURNAL OF CHEMICAL PHYSICS **122**, 184714 (2005).
- [05-11] G.Chillemi, V.Barone, P.D'Angelo, G.Mancini, I.Persson, N.Sanna, *Computational evidence for a variable first shell coordination of the cadmium (II) ion in aqueous solution*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 9186-9193 (2005).
- [05-12] P.D'Angelo, G.Chillemi, V.Barone, G.Mancini, N.Sanna, I.Persson, *Experimental evidence for a variable first shell coordination of the cadmium (II) ion in aqueous solution*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 9178-9185 (2005).
- [05-13] C.Benzi, M.Cossi, R.Improta, V.Barone, *Building cavities in a fluid or ord-like particles: a contribution to the salvation free energy in isotropic and anisotropic polarizable continuum method*, JOURNAL OF COMPUTATIONAL CHEMISTRY **26**, 1096-1105 (2005).
- [05-14] V.Barone, P.Carbonniere, C.Pouchan, *Accurate vibrational spectra and magnetic properties of organic free radicals. The case of H₂CN*, JOURNAL OF CHEMICAL PHYSICS, 122, 224308 (2005).

[05-15] D.Begue, P.Carbonniere, V.Barone, C.Pouchan, *Vibrational spectra of difluorosilane from a hybrid ab-initio and DFT quartic force field*, CHEMICAL PHYSICS LETTERS **415**, 25-29 (2005).

[05-16] V.Barone, A.Polimeno, *La chimica teorica e computazionale in Italia*, La Chimica e l'Industria **87**, 20-25 (2005).

[05-17] A.L.Piccinelli, O.Cuesta-Rubio, M.Barrios Chica, N.Mahmood, B.Pagano, M.Pavone, V.Barone, L.Rastrelli, *Structural revision of epimers clusianone and 7-epi-clusianone and anti-HIV activity of polyisoprenylated benzophenones*, TETRAHEDRON **61**, 8206-8211 (2005).

[05-18] N.Sanna, G.Chillemi, A.Grandi, S.Castelli, A.Desideri, V.Barone, *New hints on the pH driven tautomeric equilibria of the topotecan anti-cancer drug in aqueous solutions from an integrated spectroscopic and quantum-mechanical approach*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **127**, 15429-15436 (2005).

[05-19] C.Benzi, M.Cossi, V.Barone, *Accurate prediction of electronic paramagnetic spin tensors for spin probes dissolved in liquid crystals*, JOURNAL OF CHEMICAL PHYSICS **123**, 194909 (2005).

[05-20] D.Begue, P.Carbonniere, V.Barone, C.Pouchan, *Performance of ab-initio and DFT PCM methods in calculating vibrational spectra in solution: formaldehyde in acetonitrile as a test case*, CHEMICAL PHYSICS LETTERS **416**, 206-211 (2005).

[05-21] F.Costanzo, R.G. Della Valle, V.Barone, *MD simulation of the Na⁺-phenylalanine complex in water: competition between cation-π interaction and aqueous salvation*, JOURNAL OF PHYSICAL CHEMISTRY B **109**, 23016-23023 (2005).

[05-22] V.Barone, R.G.Viglione, *Harmonic and anharmonic contributions to parity-violating vibrational frequency difference between enantiomers of chiral molecules*, JOURNAL OF CHEMICAL PHYSICS **123**, 234304 (2005).

2004

[04-01] R.Improta, V.Barone, *Interplay of Electronic, Environmental, and Vibrational Effects in Determining the Magnetic Properties of Organic Free Radicals*, CHEMICAL REVIEWS **104**, 1231-1253 (2004).

[04-02] G.Scalmani, V.Barone, K.N.Kudin, C.S.Pomelli, G.E.Scuseria, M.J.Frisch, *Achieving Linear Scaling Computational Cost for the Polarizable Continuum Model of Solvation*, THEORETICAL CHEMISTRY ACCOUNTS **111**, 90-100 (2004).

[04-03] V.Barone, R.Improta, N.Regia, *Computation of protein pK's by an integrated DFT/PCM approach*, THEORETICAL CHEMISTRY ACCOUNTS **111**, 237-245 (2004).

[04-04] V.Barone, *Vibrational spectra of large molecules by density functional computations beyond the harmonic approximation. The case of pyrrole and furan*, CHEMICAL PHYSICS LETTERS **383**, 528-532 (2004).

- [04-05] V.Barone, *Vibrational zero point energies and thermodynamic functions beyond the harmonic approximation*, JOURNAL OF CHEMICAL PHYSICS **120**, 3059-3065 (2004).
- [04-06] M.Pavone, V.Barone, I.Ciofini, C.Adamo, *First-principle molecular dynamics of the Berry pseudorotation: insights on ^{19}F NMR in SF_4* , JOURNAL OF CHEMICAL PHYSICS **120**, 9167-9174 (2004).
- [04-07] C.Benzi, M.Cossi, V.Barone, *Accurate calculation of the proton magnetic shieldings in a calcium binding peptide*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **6**, 2557-2562 (2004).
- [04-08] V.Barone, *Vibrational spectra of large molecules by density functional computations beyond the harmonic approximation. The case of azabenzenes*, JOURNAL OF PHYSICAL CHEMISTRY A **108**, 4146-4150 (2004).
- [04-09] V.Barone, A.Grandi, N.Sanna, *Vibrational spectra of large molecules by density functional computations beyond the harmonic approximation. The case of uracil and 2-thiouracil*, CHEMICAL PHYSICS LETTERS **388**, 279-283 (2004).
- [04-10] P.Cimino, R.Improta, G.Bifulco, R.Riccio, L.Gomez-Paloma, V.Barone, *Nucleophilic cyclopropane ring opening in Duocarmycin SA derivatives by methanol under acid conditions: a quantum mechanical study in gas phase and in solution*, JOURNAL OF ORGANIC CHEMISTRY **69**, 2816-2824 (2004).
- [04-11] O.Crescenzi, G.Correale, A.Bolognese, V.Piscopo, M.Parrilli,V.Barone, *Observed and calculated ^1H - and ^{13}C -NMR chemical shifts of substituted 5H-pyrido[3,2-a]- and 5H-pyrido[2,3-a]phenoxazin-5-ones and of some 3H-phenoxazin-3-one derivatives*, ORGANIC AND BIOMOLECULAR CHEMISTRY **2**, 1577-1581 (2004).
- [04-12] R.Improta, V.Barone, *Assessing the reliability of density functional methods in the conformational study of polypeptides: the treatment of intra-residue non bonding interactions*, JOURNAL OF COMPUTATIONAL CHEMISTRY **25**, 1333-1341 (2004).
- [04-13] U.Cosentino, D.Pitea, G.Moro, V.Barone, A.Villa, R.N.Muller, F.Botteman, *Theoretical investigation into the influence of conformational equilibria on the water-exchange process in magnetic resonance imaging contrast agents*, THEORETICAL CHEMISTRY ACCOUNTS **111**, 204-209 (2004).
- [04-14] M.E.Alikhani, V.Barone, *Hydrogen bonding between the hydrogen peroxide molecule and the hydroperoxy radical (H_2O_2 - HO_2): the global minimum*, CHEMICAL PHYSICS LETTERS **391**, 134-137 (2004).
- [04-15] P.Carbonniere, V.Barone, *Coriolis couplings in variational computations of vibrational spectra beyond the harmonic approximation. Implementation and validation*, CHEMICAL PHYSICS LETTERS **392**, 365-371 (2004).
- [04-16] A.Bolognese, G.Correale, M.Manfra, A.Lavecchia, O.Mazzoni, E.Novellino, V.Barone, *Reaction between quinone and thiazolidine. A study on the formation mechanism of new antiproliferative quinolindiones*, TETRAHEDRON **60**, 8189-8197 (2004).

[04-17] C. Benzi, O.Crescenzi, M.Pavone, V.Barone, *Reliable NMR chemical shifts for molecules of biological interest in condensed phases by methods rooted in the density functional theory*, MAGNETIC RESONANCE IN CHEMISTRY **42**, S57-S67 (2004).

[04-18] M.Pavone, C.Benzi, F.De Angelis, V.Barone, *Hyperfine coupling constants of dimethyl-nitroxide in aqueous solution: Car-Parrinello molecular dynamics and discrete-continuum approaches*, CHEMICAL PHYSICS LETTERS **395**, 120-126 (2004).

[04-19] A.Bolognese, G.Correale, M.Manfra, A.Lavecchia, E.Novellino, V.Barone, *Thiazolidin-4-one formation. Mechanistic and synthetic aspects of the reaction of imine and mercaptoacetic acid under microwave and conventional heating*, ORGANIC AND BIOMOLECULAR CHEMISTRY **2**, 2809-2813 (2004).

[04-20] I.Ciofini, V.Barone, C.Adamo, *Complete structural and magnetic characterization of biological radicals in solution by an integrated quantum mechanical approach. Glycyl radical as a case study*, JOURNAL OF CHEMICAL PHYSICS **121**, 6710-6718 (2004).

[04-21] P.Cimino, L.Gomez Paloma, V.Barone, *Regioselectivity and nucleophilic control in the cyclopropane ring opening of Duocarmycin SA derivatives under neutral and acid conditions: a quantum mechanical study in gas-phase and in solution*, JOURNAL OF ORGANIC CHEMISTRY **69**, 7414-7422 (2004).

[04-22] R.Improta, V.Barone, *Absorption and fluorescence spectra of uracil in the gas phase and in aqueous solution: a quantum mechanical study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **126**, 14320-14321 (2004).

[04-23] P.Carbonniere, V.Barone, *Performances of different density functionals in the computation of vibrational spectra beyond the harmonic approximation*, CHEMICAL PHYSICS LETTERS **399**, 226-229 (2004).

[04-24] E.Langella, R.Improta, V.Barone, *Checking the pH-induced conformational transition of prion protein by molecular dynamics simulations: effect of protonation of histidine residues*, BIOPHYSICAL JOURNAL **87**, 3623-3632 (2004).

[04-25] M.D'Amore, F.Auriemma, C.De Rosa, V.Barone, *Disordered chain conformations of polytetrafluoroethylene in the high temperature crystalline form I*, MACROMOLECULES **37**, 9473-9480 (2004).

2003

[03-01] G.Talarico, V.Barone, L.Joubert, C.Adamo, *A general computational strategy to study polymerization reactions at aluminum based catalysts*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **91**, 474-482 (2003).

[03-02] M.Cossi, N.Regia, G.Scalmani, V.Barone, *Energies, Structures, and Electronic Properties of Molecules in Solution by the C-PCM Solvation Model*, JOURNAL OF COMPUTATIONAL CHEMISTRY **24**, 669-681 (2003).

[03-03] F.Aquilante, M.Cossi, O.Crescenzi, V.Barone, *Computation of the Acetone UV Spectrum in Gas Phase and in Aqueous Solution by a Mixed Discrete/Continuum Model*, MOLECULAR PHYSICS **101**, 1945-1953 (2003).

[03-04] M.C.Menziani, P.G. de Benedetti, E.Langella, V.Barone, *Seeking for binding determinants of the prion protein in human plasminogen*, MOLECULAR PHYSICS **101**, 2763-2773 (2003).

[03-05] G.A.A.Saracino, R.Improta, G.Scalmani, V.Barone, *Absolute pK_a determination for carboxylic acids using Density Functional Theory and Polarizable Continuum Model* CHEMICAL PHYSICS LETTERS **373**, 411-415 (2003).

[03-06] M.d'Amore, R.Improta, V.Barone, *Conformational Behavior and Magnetic Properties of a Nitroxide Dipeptide Analogue in Vacuo and in Aqueous Solution*, JOURNAL OF PHYSICAL CHEMISTRY A **107**, 6264-6269 (2003).

[03-07] V.Barone, A.Palma, N.Sanna, *Toward a reliable computational support to the spectroscopic characterization of excited state intramolecular proton transfer: [2,2'-bipyridine]-3,3'-diol as a test case*, CHEMICAL PHYSICS LETTERS **381**, 451-457 (2003).

[03-08] F.Aquilante, V.Barone, B.O.Roos, *A theoretical investigation of valence and Rydberg electronic states of acrolein*, JOURNAL OF CHEMICAL PHYSICS **119**, 12323-12334 (2003).

2002

[02-01] C.Benzi, R.Improta, G.Scalmani, V.Barone, *A quantum mechanical study of the conformational behavior of proline and 4R-hydroxyproline dipeptide analogues in vacuo and in aqueous solution*, JOURNAL OF COMPUTATIONAL CHEMISTRY **23**, 1-10 (2002)

[02-02] R.Improta, V.Barone, K.N.Kudin, G.E.Scuseria, *Structure and magnetic properties of nitroxide molecular crystals by density functional calculations employing periodic boundary conditions*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 113-120 (2002).

[02-03] P.D'Angelo, V.Barone, G.Chillemi, N.Sanna, W.Meyer-Klaucke, N.V.Pavel, *Hydrogen and higher shell contributions in Zn^{2+} , Ni^{2+} , and Co^{2+} aqueous solution: an x-ray absorption fine structure and molecular dynamics study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 1958-1967 (2002).

[02-04] G.Chillemi, P.D'Angelo, N.V.Pavel, N.Sanna, V.Barone, *Development and validation of an integrated computational approach for the study of ionic species in solution by means of effective two-body potentials. The case of Zn^{2+} , Ni^{2+} , and Co^{2+} in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 1968-1976 (2002).

[02-05] E.Langella, N.Regà, R.Improta, O.Crescenzi, V.Barone, *Conformational Analysis of the Tyrosine Dipeptide Analogue in the Gas Phase and in Aqueous Solution by a Density Functional / Continuum Solvent Model*, JOURNAL OF COMPUTATIONAL CHEMISTRY **23**, 650-661 (2002).

[02-06] A.M.Tedeschi, G. D'Errico, E.Busi, R.Basosi, V.Barone, *Micellar aggregation of sulfonate surfactants studied by electron spin resonance of a cationic nitroxide: an experimental and computational approach*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS **4**, 2180-2188 (2002).

[02-07] C.Adamo, V.Barone, *Physically motivated density functionals with improved accuracy: the mPBE model*, JOURNAL OF CHEMICAL PHYSICS **116**, 5933-5940 (2002).

[02-08] U.Cosentino, A.Villa, D.Pitea, G.Moro, V.Barone, A.Maiocchi, *Conformational characterization of Lanthanide(III)-DOTA complexes by ab-initio investigation in vacuo and in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 4901-4909 (2002).

[02-09] M.Cossi, G.Scalmani, N.Regia, V.Barone, *New developments in the Polarisable Continuum Model for quantum mechanical and classical calculations on molecules in solution*, JOURNAL OF CHEMICAL PHYSICS **117**, 43-54 (2002).

[02-10] R. Improta, F. Mele, O. Crescenzi, C. Benzi, V. Barone, *Understanding the Role of Stereoelectronic Effects in Determining Collagen Stability. II. A Quantum Mechanical / Molecular Mechanical Study of (Proline-Proline-Glycine)_n Polypeptides*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 7857-7865 (2002).

[02-11] V.Barone, O.Crescenzi, R.Improta, *Computation of Spectroscopic Parameters in Vacuo and in Condensed Phases by Methods Based on the Density Functional Theory*, QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIPS **21**, 105-118 (2002).

[02-12] E.Langella, R.Improta, V.Barone, *Conformational and spectroscopic analysis of the tyrosyl radical dipeptide analogue in the gas phase and in aqueous solution by a density functional/continuum solvent model*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **124**, 11531-11540 (2002).

[02-13] V.Barone, A.Bencini, D.Gatteschi, F.Totti, *DFT description of the magnetic properties and electron localization in dinuclear di- μ -oxo bridged manganese complexes*, CHEMISTRY, EUROPEAN JOURNAL **8**, 5019-5027 (2002).

[02-14] G.A.A.Saracino, A.Tedeschi, G.D'Errico, R.Improta, V.Barone, *Solvent polarity and pH effects on the magnetic properties of ionizable nitroxide radicals: a combined computational and experimental study of 2,2,5,5-tetramethyl-3,carboxy-pyrrolidine and 2,2,6,6-tetramethyl-4,carboxy-piperidine nitroxides*, JOURNAL OF PHYSICAL CHEMISTRY A **106**, 10700-10706 (2002).

[02-15].Guillemoles, V.Barone, L.Joubert, C.Adamo, *A Theoretical Investigation of the Ground and Excited States of Selected Ru and Os Polypyridyl Molecular Dyes*, JOURNAL OF PHYSICAL CHEMISTRY A **106**, 11354-11360 (2002).

[02-16] G.Scalmani, N.Regia, M.Cossi, V.Barone, *Finite Elements Molecular Surfaces in Continuum Solvent Models for Large Chemical Systems*, JOURNAL OF COMPUTATIONAL METHODS IN SCIENCES AND ENGINEERING **2**, 159-164 (2002).

[02-17] A.Bolognese, G.Correale, M.Manfra, A.Lavecchia, O.Mazzoni, E.Novellino, V.Barone, P.La Colla, R.Loddo, C.Murgioni, A.Pani, I.Serra, G.Setzu, *Antitumor agents. 1. Synthesis, Biological evaluation and molecular modeling of 5H-pyrido[3,2- α]phenoxazin-5-one, a new actynomicin D analog with potent antiproliferative activity*, JOURNAL OF MEDICINAL CHEMISTRY **45**, 5205-5216 (2002).

[02-18] A.Bolognese, G.Correale, M.Manfra, A.Lavecchia, O.Mazzoni, E.Novellino, V.Barone, P.La Colla, R.Loddo, *Antitumor agents. 2. Synthesis, Structure-Activity Relationships and Biological Evaluation of Substituted 5H-pyridophenoxazin-5-ones with Potent AntiproliferativeAactivity*, JOURNAL OF MEDICINAL CHEMISTRY **45**, 5217-5223 (2002).

2001

[01-1] C.Adamo, M.Cossi, N.Regia, V.Barone, *New computational strategies for the quantum mechanical study of biological systems in condensed phases*, in Theoretical Biochemistry. Processes and Properties of Biological Systems, L.Eriksson, Ed., Elsevier, 467-538 (2001).

[01-2] A.Di Matteo, M. di Valentin, G.Giacometti, V.Barone, *Structure and magnetic properties of aza-aromatic triplet states. The case of quinoxaline*, CHEMICAL PHYSICS LETTERS **335**, 427-434 (2001).

[01-3] R.Improta, V.Barone, K.N.Kudin, G.E.Scuseria, *Conformational behavior of polyglycine as predicted by a density functional model with periodic boundary conditions*, JOURNAL OF CHEMICAL PHYSICS **114**, 2541-2549 (2001).

[01-4] C.S.Pomelli,J.Tomasi,V.Barone, *An improved iterative solution to solve the electrostatic problem in the polarizable continuum model*, THEORETICAL CHEMISTRY ACCOUNTS **105**, 446-451 (2001).

[01-5] V.Barone, A.Bolognese, G.Correale, M.V.Diurno, I.Gomez-Monterrey, O.Mazzoni, *Intramolecular CH-O interaction between lactam oxygen and N-alkylic protons*, JOURNAL OF MOLECULAR GRAPHICS AND MODELLING **19**, 318-324 (2001).

[01-6] R.Improta, K.N.Kudin, G.E.Scuseria, V.Barone, *Structure and conformational behavior of biopolymers by density functional calculations employing periodic boundary coniditions. I. The case of poly-glycine, poly-alanine, and poly-aminoisobutirric acid*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **123**, 3311-3322 (2001).

[01-7] M.Cossi, N.Regia, M.Scalmani, V.Barone, *Polarizable dielectric model of solvation with inclusion of charge penetration effects*, JOURNAL OF CHEMICAL PHYSICS **114**, 5691-5701 (2001).

[01-8] R.Improta, G.Scalmani, V.Barone, *Quantum mechanical prediction of the magnetic titration curve of a nitroxide ‘spin probe’*, CHEMICAL PHYSICS LETTERS **336**, 349-356 (2001).

[01-9] C.Adamo, M.Heitzman, F.Meilleur, N.Regia, G.Scalmani, A.Grand, J.Cadet, V.Barone, *Interplay of intrinsic and environmental effects on the magnetic properties of free radicals issuing from H atom addition to cytosine*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **123**, 7113-7117 (2001).

[01-10] R.Improta, C.Benzi, V.Barone, *Understanding the role of stereoelectronic effects in determining collagen stability. I. A quantum mechanical study of proline, hydroxyproline and fluoroproline dipeptide analogues in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **123**, 12568-12577 (2001).

[01-11] R.Improta, V.Barone, *Structural and magnetic properties of model spin probes in aqueous solution: an application of recent developments in density functional theory and in the polarizable continuum model*, Recent Advances in Density Functional Methods, (2001).

[01-12] C.Adamo, P.H.M.Budzelaar, G.Talarico, V.Barone, *Modelling polymerization reaction at aluminum based catalysts: is DFT a reliable computational tool*, JOURNAL OF PHYSICAL CHEMISTRY A **105**, 9014-9023 (2001).

[01-13] M.Cossi, V.Barone, *Time-dependent density functional theory for molecules in liquid solutions*, JOURNAL OF CHEMICAL PHYSICS **115**, 4708-4717 (2001).

[01-14] V.Barone, F.Fabrizi de Biani, E.Ruiz, B.Sieklucka, *Electron transfer in the $[Pt(NH_3)_4]^{2+}$ $[W(CN)_8]^{3-}$ donor-acceptor system. The environment effect: a time dependent density functional study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **123**, 10742-10743 (2001).

[01-15] R.Improta, N.Regia, C.Aleman, V.Barone, *Conformational behavior of macromolecules in solution by the polarizable continuum model in quantum mechanical and molecular mechanical frames. Homopolypeptides of α -aminoisobutyric acid as test cases*, MACROMOLECULES **134**, 7550-7559 (2001).

2000

[00-01] G.Scalmani, J.Brèdas, V.Barone, *Ab-initio Prediction of the Gas-Phase Structure and Electronic Properties of $M-CH_3$ ($M=Li,Na$) and $M-CCH$ ($M=Li,Na,K$): a Combined post-HF and DFT Study*, JOURNAL OF CHEMICAL PHYSICS, **112**, 1178-1191 (2000).

[00-02] R.Arnaud,C.Adamo,M.Cossi,A.Milet,Y.Vallee,V.Barone, *Theoretical Study of the Addition of Hydrogen Cyanide to Methanimine in the Gas Phase and in aqueous Solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **122**, 324-330 (2000).

[00-03] M.Cossi, V.Barone, *Solvent effect on vertical electronic transitions by the polarizable continuum model*, JOURNAL OF CHEMICAL PHYSICS, **112**, 2427-2435 (2000).

[00-04] P.A.Nielsen, P.O.Norrby, T.Liljefors, N.Regia, V.Barone, *Quantum mechanical conformatational analysys of β -alanine zwitterion in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **122**, 3151-3155 (2000).

[00-05] R.Improta, A.di Matteo, V.Barone, *Effective modeling of intrinsic and environmental effects on the structure and EPR parameters of nitroxides by an integrated QM/MM/PCM approach*, THEORETICAL CHEMISTRY ACCOUNTS, **104**, 273-279 (2000).

[00-06] F.Illas, I.de P.R.Moreira, C.de Graaf, V.Barone, *Magnetic coupling in biradicals, binuclear complexes and wide gap insulators: a survey of ab-initio wave function and density functional theory approaches*, THEORETICAL CHEMISTRY ACCOUNTS, **104**, 265-272 (2000).

[00-07] C.Adamo, V.Barone, R.Subra, *On the mechanism of spin polarization in aromatic free radicals*, THEORETICAL CHEMISTRY ACCOUNTS, **104**, 207-209 (2000).

- [00-08] R.Arnaud, V.Vetere, V.Barone, *Regioselectivity of Radical Additions to Substituted Olefins: a Density Functional Study*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **21**, 675-691 (2000).
- [00-09] U.Cosentino, A.Villa, D.Pitea, G.Moro, V.Barone, *Extension of computational chemistry to the study of Lanthanide (III) ions in aqueous solution: implementation and validation of the continuum solvent approach*, JOURNAL OF PHYSICAL CHEMISTRY B **104**, 8001-8007 (2000).
- [00-10] L.Gagliardi, S.Evangelisti, V.Barone, B.Roos, *On the dissociation of N_6 into 3 N_2 molecules*, CHEMICAL PHYSICS LETTERS, **320**, 518-522 (2000).
- [00-11] L.Gagliardi, C.K.Skylaris, A.Willets, J.M.Dyke, V.Barone, *A density functional study of thorium halides*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **2**, 3111-3114 (2000).
- [00-12] C.Adamo, V.Barone, *Structures and properties of lanthanide and actinide complexes by a new density functional approach. Lanthanum, gadolinium, lutetium and thorium halides as case studies*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **21**, 1153-1166 (2000).
- [00-13] R.Improta, G.Scalmani, V.Barone, *Radical cations of DNA bases: some insights on structure and fragmentation patterns by density functional methods*, INTERNATIONAL JOURNAL OF MASS SPECTROMETRY, **201**, 321-336 (2000).
- [00-14] M.Cossi, V.Barone, *Separation between fast and slow polarizations in continuum solvation models*, JOURNAL OF PHYSICAL CHEMISTRY A, **104**, 10614-10622 (2000).
- [00-15] G.Talarico, P.H.M.Budzelaar, V.Barone, C.Adamo, *A theoretical study of the competition between ethylene insertion and chain transfer in cationic aluminum systems*, CHEMICAL PHYSICS LETTERS, **329**, 99-105 (2000).
- [00-16] M.Cossi, V.Barone, *Solvent Effects by Effective Hamiltonian Model*, in European Summerschool in quantum chemistry, B.O.Roos and P.-O. Widmark, Editors, Lund University, **2**, 551-597 (2000).
- [00-17] V.Aquilanti, G.Capecchi, S.Cavalli, C.Adamo, V.Barone, *Representation of potential energy surfaces by discrete polynomials: proton transfer in malonaldehyde*, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, **2**, 4095-4103 (2000).
- [00-18] F.De Angelis, A.Sgamellotti, M.Cossi, N.Regia, V.Barone, *A plane wave implementation of the polarizable continuum model*, CHEMICAL PHYSICS LETTERS, **328**, 302-309 (2000).
- [00-19] C.Adamo, V.Barone, *A TDDFT study of the electronic spectrum of s-tetrazine in the gas-phase and in aqueous solution*, CHEMICAL PHYSICS LETTER, **330**, 152-160 (2000).
- [00-20] C.Adamo, V.Barone, *Inexpensive and accurate predictions of optical excitations in transition-metal complexes: the TDDFT/PBE0 route*, THEORETICAL CHEMISTRY ACCOUNTS, **105**, 169-172 (2000).

- [99-1] V.Barone,N.Regia,T.Bally,G.N.Sastry, *The Ring Opening Reaction of Cyclobutene Radical Cation: the Effect of Solvent on Competing Pathways*, JOURNAL OF PHYSICAL CHEMISTRY A, **103**, 217-219 (1999).
- [99-2] F. Jolibois, A.Grand, J.Cadet, C.Adamo, V.Barone, *Towards an effective computational protocol for the study of radiation damage in DNA bases. H addition to thymine as a test case*, CHEMICAL PHYSICS LETTERS, **301**, 255-262 (1999).
- [99-3] G.Scalmani,V.Barone, *Use of molecular symmetry in the computation of solvation energies and their analytical derivatives by the polarizable continuum model*, CHEMICAL PHYSICS LETTERS, **301**, 263-269 (1999).
- [99-5] V.Barone, A.di Matteo, F.Mele, I.de P.R. Moreira, F.Illas, *Through Bond and through Space Effects in the Magnetic Properties of Nitroxide Biradicals by an Integrated QM/MM Approach Including Solvent Effects*, CHEMICAL PHYSICS LETTERS, **302**, 240-248 (1999).
- [99-6] C.Adamo,A.di Matteo,P.Rey,V.Barone, *Tuning of Structural and Magnetic Properties of Nitronylnitroxides by the Environment. A Combined Experimental and Computational Study*, JOURNAL OF PHYSICAL CHEMISTRY A **103**, 3481-3488 (1999).
- [99-7] C.Adamo, V.Barone, A.Bencini, F.Totti, I.Ciofini, *On Calculation and Modeling Magnetic Exchange Interactions in Weakly Bonded Systems. The Case of the Ferromagnetic Copper(II) μ_2 -Azido Bridged Complexes*, INORGANIC CHEMISTRY **38**, 1996-2004 (1999).
- [99-8] V.Barone,A.Bencini,I.Ciofini,C.Daul, *Structure and Magnetic Properties of Oxoverdazyl Radicals and Biradicals by an Integrated Computational Approach*, JOURNAL OF PHYSICAL CHEMISTRY A **103**, 4275-4282 (1999).
- [99-9] N.Regia,M.Cossi,V.Barone,C.S.Pomelli,J.Tomasi, *Toward an Effective and Reliable Representation of Solvent Effects in the Study of Biochemical Systems*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **73**, 219-227 (1999).
- [99-10] S.Fliszàr, E.C.Vauthier,V.Barone, *Core and Valence Electrons in Atom-by-atom Descriptions of Molecules*, ADVANCES IN QUANTUM CHEMISTRY, **36**, 27-44 (1999).
- [99-11] C.Adamo, A.di Matteo,V.Barone, *From Classical Density functionals to Adiabatic Connection Methods. The State of the Art*, ADVANCES IN QUANTUM CHEMISTRY, **36**, 45-76 (1999).
- [99-12] C.Adamo, M.Cossi, G.Scalmani,V.Barone, *Accurate Static Polarizabilities by Density Functional Theory: Assessment of the PBE0 Model*, CHEMICAL PHYSICS LETTERS, **307**, 265-271 (1999).
- [99-13] N.Regia,M.Cossi,V.Barone, *Improving Performance of Polarizable Continuum Model for Study of Large Molecules in Solution*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **20**, 1186-1198 (1999).
- [99-14] A.di Matteo,C.Adamo, M.Cossi, P.Rey, V.Barone, *Intrinsic and Environmental Effects in the Physico-Chemical Properties of Nitroxides. The case of 2-phenyl-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazol-1-oxyl-3-oxide*, CHEMICAL PHYSICS LETTERS, **310**, 159-165 (1999).

- [99-15] A.di Matteo,V.Barone, *Development and Validation of Effective Computational strategies for the Study of Metal-Nitroxide systems*, JOURNAL OF PHYSICAL CHEMISTRY A, **103**, 7676-7685 (1999).
- [99-16] C.Adamo,R.Arnaud,G.Scalmani,H.Mueller,F.Sahli,V.Barone, *Theoretical Study of a new Building Block for Organic Conductors: Tetrathiapentalene and its Radical Cation*, JOURNAL OF PHYSICAL CHEMISTRY B, **103**, 6863-6869 (1999).
- [99-17] M.Cossi,V.Barone,M.Robb, *A Direct Procedure for the Evaluation of Solvent Effects in MC-SCF Calculations*, JOURNAL OF CHEMICAL PHYSICS, **111**, 5295-5302 (1999).
- [99-18] M.Bienati,C.Adamo,V.Barone, *Performance of a new hybrid Hartree-Fock / Kohn-Sham model (B98) in predicting vibrational frequencies, polarisabilities and NMR chemical shifts*, CHEMICAL PHYSICS LETTERS, **311**, 69-76 (1999).
- [99-19] C.Adamo,G.Scuseria,V.Barone, *Accurate Excitation Energies from Time-Dependent Density Functional Theory: Assessing the PBE0 Model*, JOURNAL OF CHEMICAL PHYSICS, **111**, 2889-2899 (1999).
- [99-20] M.d'Ischia, N.Regia,V.Barone, *Medium-dependent Competitive Pathways in the Reactions of Polyunsaturated Fatty Acids with Nitric Oxide in the Presence of Oxygen. Structural Characterisation of Nitration Products and a Theoretical Mechanistic Insight*, TETRAHEDRON, **55**, 9297-9308 (1999).
- [99-21] C.Adamo,V.Barone, *Accurate excitation energies from time-dependent density functional theory: assessing the PBE0 model for organic free radicals*, CHEMICAL PHYSICS LETTERS, **314**, 152-157 (1999).
- [99-22] C.Adamo, M.Cossi, V.Barone, *An Accurate Density-Functional Method for the Study of Magnetic Properties. The PBE0 Model*, THEOCHEM, **493**, 145-157 (1999).
- [99-23] C.S.Pomelli,J.Tomasi,M.Cossi,V.Barone, *Effective Generation of Molecular Cavities in the Polarizable Continuum Model by the DefPol Procedure*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **20**, 1693-1701 (1999).

1998

- [98-1] V.Barone, M.Cossi, J.Tomasi, *Geometry Optimization of Molecular Structures in Solution by the Polarizable Continuum Model*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **19**, 407-417 (1998).
- [98-2] C.Adamo,V.Barone, *Exchange functionals with improved long range behaviour and adiabatic connection methods without adjustable parameters. The mPW and mPW1PW models*, JOURNAL OF CHEMICAL PHYSICS, **108**, 627-631 (1998).
- [98-3] C.Adamo,V.Barone, *Implementation and validation of the Lacks-Gordon exchange functional in conventional density functional and adiabatic connection methods*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **19**, 418-429 (1998).

[98-4] V.Barone,M.Cossi, *Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model*, JOURNAL OF PHYSICAL CHEMISTRY A, **102**, 1995-2001 (1998).

[98-5] F.Jolibois, J.Cadet, A.Grand, R.Subra, V.Barone, N.Regia, *Structures and spectroscopic characteristics of 5,6-dihydro-6-thymyl and 5,6-dihydro-5-thymyl radicals by an integrated approach including electronic, vibrational and solvent effects*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **120**, 1864-1871 (1998).

[98-6] M.Cossi,V.Barone, B.Mennucci, J.Tomasi, *Ab-initio Study of Ionic Solutions by a Polarizable Continuum Dielectric Model*, CHEMICAL PHYSICS LETTERS, **286**, 253-260 (1998).

[98-7] V.Barone,A.Bencini,I.Ciofini,C.A.Daul,F.Totti, *Density Functional Modeling of Double Exchange Interactions in Transition Metal Complexes. Calculation of the Ground and Excited State Properties of $[Fe_2(OH)_3(tmatcn)_2]^{2+}$* , JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **120**, 8357-8365 (1998).

[98-8] R.Arnaud, N.Bugaud, V.Vetere, V.Barone, *Role of Polar and Enthalpic Effects in the Addition of Methyl Radical to Substituted Alkenes: a Density-Functional Study Including Solvent Effects*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **120**, 5733-5740 (1998).

[98-9] N.Regia, M.Cossi, V.Barone, *Structure and Magnetic Properties of Glycine Radical in Solution at Different pH Values*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **120**, 5723-5732 (1998).

[98-10] N.Regia,M.Cossi,V.Barone, *Towards Linear Scaling in Continuum Solvent Models: a New Iterative Procedure for Energies and Geometry Optimizations*, CHEMICAL PHYSICS LETTERS, **293**, 221-229 (1998).

[98-11] V.Barone, A.Bencini, M.Cossi, A.di Matteo,M.Mattesini, F.Totti, *Assessment of a combined QM/MM approach for the study of large nitroxide systems in vacuo and in condensed phases*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **120**, 7069-7078 (1998).

[98-12] G.Schuurman, M.Cossi, V.Barone, J.Tomasi, *Prediction of pKa Using ab-initio Continuum Solvation Quantum Chemistry. I.Application of PCM-UATM for Carboxylic Acids*, JOURNAL OF PHYSICAL CHEMISTRY A, **102**, 6706-6712 (1998).

[98-13] M.Cossi,V.Barone, *Analytical Second Derivatives of the Free Energy in Solution by Polarizable Continuum models*, JOURNAL OF CHEMICAL PHYSICS, **109**, 6246-6254 (1998).

[98-14] R.Arnaud, V.Vetere, V.Barone, *Regioselectivity of Methyl Radical Addition to Fluoroethenes: a Quantum Mechanical Study*, CHEMICAL PHYSICS LETTERS, **293**, 295-301 (1998).

[98-15] C.Adamo, R.Subra, A.di Matteo, V.Barone, *Structure and Magnetic Properties of Benzyl, Anilino, and Phenoxy Radicals by Density Functional Calculations Including Vibrational Averaging and Solvent Effects*, JOURNAL OF CHEMICAL PHYSICS, **109**, 10244-10255 (1998).

[98-16] M.Cossi,C.Adamo,V.Barone, *Solvent effects on the profile of an SN2 reaction*, CHEMICAL PHYSICS LETTERS, **297**, 1-7 (1998).

[98-17] R.Arnaud,R.Subra,V.Barone, *A Theoretical Study of Substituent Effects on the Structure of Isolated and Condensed three-membered Rings. A Comparison between Radicals and Parent Hydrocarbons*, THEORETICAL CHEMISTRY ACCOUNTS, **99**, 411-419 (1998).

[98-18] C.Amovilli, V.Barone, R.Cammi, E.Cances, M.Cossi, B.Mennucci, C.S.Pomelli, J.Tomasi, *Recent Advances in the Description of Solvent Effects with the Polarizable Continuum Model*, ADVANCES IN QUANTUM CHEMISTRY, **32**, 227-262 (1998).

[98-19] C.Adamo,V.Barone, *Toward Chemical Accuracy in the Computation of NMR Shieldings: the PBE0 Model*, CHEMICAL PHYSICS LETTERS, **298**, 113-119 (1998).

1997

[97-1] V.Barone, A.Bencini, F.Totti, M.G.Uytterhoeven, *Comparison between post-HF and DFT Methods for the Study of Strength and Mechanism of Cleavage of Hg-C Bond*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **61**, 361-367 (1997).

[97-2] V.Barone, C.Adamo, *Towards a General Protocol for the Study of static and Dynamic Properties of Hydrogen-Bonded Systems*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **61**, 429-442 (1997).

[97-3] V.Barone, C.Adamo, *First-Row Transition Metal Hydrides: a Challenging Playground for New Theoretical Approaches*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **61**, 443-451 (1997).

[97-4] C.Adamo,V.Barone, *Structural and Dynamical Features of Hydrogen Bonds from Conventional and Hybrid Density Functional Methods* in Recent Advances in Density Functional Methods (Part II), edited by D.P.Chong, World Scientific Publishing Co., pp.115-164 (1997).

[97-5] V.Barone, R.Arnaud, *Diels-Alder Reactions: an Assessment of Quantum Mechanical Procedures*, JOURNAL OF CHEMICAL PHYSICS, **106**, 8727-8732 (1997).

[97-6] Y.Vallee, P.Y.Chauvant, S.Pinet, N.Pelloux-Leon, R.Arnaud, V.Barone, *[4π+2π] Cycloadditions of N-Acyl-Thioformamides*, PHOSPHOROUS, SULFUR, AND SILICON, **120**, 245-258 (1997).

[97-7] V.Barone, M.Cossi, J.Tomasi, *A New Definition of Cavities for the Computation of Solvation Free Energies by the Polarizable Continuum Model*, JOURNAL OF CHEMICAL PHYSICS, **107**, 3210-3221 (1997).

[97-8] C.Adamo,V.Barone, *Towards Reliable Adiabatic Connection Models Free from Adjustable Parameters*, CHEMICAL PHYSICS LETTERS, **274**, 242-250 (1997).

[97-9] V.Barone, G.Capecci,Y.Brunel, M.L.Dheu, R.Subra, *Development and Validation of Force Field Parameters for Molecular Simulations of Peptides and Proteins Containing Open-Shell Residues*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **18**, 1720-1728 (1997).

[97-10] A.Bencini, F.Totti, C.Daul, K.Doclo, P.Fantucci, V.Barone, *Density Functional Calculations of Magnetic Exchange Interactions in Polynuclear Transition Metal Complexes*, INORGANIC CHEMISTRY, **36**, 5022-5030 (1997).

[97-11] V.Barone, A.Bencini, A.di Matteo, *Intrinsic and Environmental Effects in the Structure and Magnetic Properties of Organic Molecular Magnets. The case of bis(imino)nitroxide*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **119**, 10831-10837 (1997).

[97-12] C.Adamo, M.Cossi, V.Barone, *Catalytic and Bulk Solvent Effects on Proton Transfer. Formamide as a Case Study*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **18**, 1993-2000 (1997).

[97-13] N.Regia,M.Cossi,V.Barone, *Intrinsic and environmental effects in the structure and magnetic properties of glycine radical in aqueous solution*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **119**, 12962-12967 (1997).

1996

[96-1] V.Barone, C.Adamo, *Validation of Hybrid Density Functional/ Hartree-Fock Approaches for the Study of Homogeneous Catalysis*, JOURNAL OF PHYSICAL CHEMISTRY **100**, 2094-2099 (1996).

[96-2] V.Barone, C.Adamo, F.Mele, *Comparison of Conventional and Hybrid Density Functional Approaches. Cationic Hydrides of First-Row Transition Metals as a Case Study*, CHEMICAL PHYSICS LETTERS, **249**, 290-296 (1996).

[96-3] V.Barone, R.Subra, *Structure and Hyperfine Parameters of Cyclopropyl and Bicyclobutyl Radicals from post-Hartree-Fock computations*, JOURNAL OF CHEMICAL PHYSICS, **104**, 2630-2637 (1996).

[96-4] V.Barone, A.Grand, C.Minichino, R.Subra, *Vibrational Modulation Effects in EPR Spectra*, in Strategies and Applications in Quantum Chemistry, Y.Ellinger, M.De Franceschi, Eds., Kluwer (1996), p.251.

[96-5] V.Barone, A.Bencini, F.Totti, M.G.Uytterhoeven, *Theoretical Characterization of the Mechanism of Hg-C Bond Cleavage by Halogenic Acids*, ORGANOMETALLICS, **15**, 1465-1469 (1996).

[96-6] V.Barone, R.Arnaud, *Study of Prototypical Diels-Alder Reactions by a Hybrid Density Functional/ Hartree-Fock Approach*, CHEMICAL PHYSICS LETTERS, **251**, 393-399 (1996).

[96-7] M.Cossi, V.Barone, R.Cammi, J.Tomasi, *Ab-initio Study of Solvated Molecules: a New Implementation of the Polarizable Continuum Model*, CHEMICAL PHYSICS LETTERS, **255**, 327-335 (1996).

[96-8] V.Barone, R.Arnaud, P.Y.Chavant,Y.Vallee, *Substituent Effects in the Hetero Diels-Alder Reaction of Thiocarbonyl Compounds with Butadiene*, JOURNAL OF ORGANIC CHEMISTRY, **61**, 5121-5129 (1996).

[96-9] V.Barone, C.Adamo, Y.Brunel, R.Subra, *Structures, Hyperfine Parameters and Inversion Barriers of Cyclopropyl and Oxiranyl Radicals*, JOURNAL OF CHEMICAL PHYSICS, **105**, 3168-3174 (1996).

[96-10] R.Caputo, M.De Nisco, G.Palumbo, C.Adamo, V.Barone, *Semiempirical Study of the Aromatic Ring Bromination in 1,4-Benzothiazines, 1,4-Benzoxathianes, and 1,4-Benzodithianes*, GAZZETTA CHIMICA ITALIANA, **126**, 595-598 (1996).

[96-11] V.Barone, *Electronic, Vibrational and Environmental Effects on the Hyperfine Constants of Nitroxide Radicals. H₂NO as a Case Study*, CHEMICAL PHYSICS LETTERS, **262**, 201-206 (1996).

[96-12] C.Adamo, V.Dillet, V.Barone, *Solvent Effects on the Conformational Behaviour of Model Peptides. A Comparison Between Different Continuum Models*, CHEMICAL PHYSICS LETTERS, **263**, 113-118 (1996).

[96-13] V.Barone, C.Adamo, *Proton Transfer in the Ground and Lowest Excited States of Malonaldehyde. A Comparative Density Functional and Post Hartree-Fock Study*, JOURNAL OF CHEMICAL PHYSICS, **105**, 11007-11019 (1996).

[96-14] N.Regia, M.Cossi,V.Barone, *Development and Validation of Reliable Quantum Mechanical Approaches for the Study of Free Radicals in Solution*, JOURNAL OF CHEMICAL PHYSICS, **105**, 11060-11067 (1996).

[96-15] V.Barone,S.Fliszár, *Applications of Density Functional Theory Approaching Chemical Accuracy to the Study of Typical Carbon-Carbon and Carbon-Hydrogen Bonds*, THEOCHEM, **369**, 29-37 (1996).

1995

[95-1] V.Barone,C.Minichino, *From Concepts to Algorithms for the Treatment of Large Amplitude Internal Motions and Unimolecular Reaction Rates*, THEOCHEM, **330**, 365-376 (1995).

[95-2] V.Barone,C.Adamo,C.Minichino, *Direct Catalytic Effect and Fine Modulation of Solvent in the Keto-Enol Isomerization of Amides*, THEOCHEM, **330**, 325-333(1995).

[95-3] V.Barone, C.Adamo, F.Lelj, *Conformational Behaviour of Gaseous Glycine by a Density Functional Approach*, JOURNAL OF CHEMICAL PHYSICS, **102**, 366-370 (1995).

[95-4] C.Adamo,V.Barone,A.Fortunelli, *Validation of Self-consistent Hybrid Density Functionals for the Study of Structural and Electronic Characteristics of Organic π-Radicals*, JOURNAL OF CHEMICAL PHYSICS, **102**, 384-392 (1995).

[95-5] V.Barone, *Validation of self-consistent hybrid approaches for the study of transition metal complexes. NiCO and CuCO as test cases*, CHEMICAL PHYSICS LETTERS, **233**, 129-133 (1995).

[95-6] V. Barone, C. Adamo, A. Grand, Y. Brunel, M.Fontecave, R. Subra, *Conformational Behaviour and Magnetic Properties of Organic Radicals Derived from Aminoacid Residues. The Dipeptide Analogue of Glycine Radical*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **117**, 1083-1089 (1995).

[95-7] V.Barone, *Structure, EPR Parameters, and Reactivity of Organic Free Radicals from a Density Functional Approach*, THEORETICA CHIMICA ACTA, **91**, 113-128 (1995).

[95-8] V.Barone, A.Bolognese, M.Buonanno, *Photochemical Behaviour of Some Substituted Benzophenoxazinones*, JOURNAL OF HETEROCYCLIC CHEMISTRY **32**, 743-746 (1995).

- [95-9] V.Barone, S.Fliszár, *Theoretical Energies of Representative Carbon-Carbon Bonds*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **55**, 469-476 (1995).
- [95-10] V.Barone, P.Milano, L.Orlandini, C.Adamo, *Proton transfer in the ground and excited electronic states of [2,2'-bipyridyl]-3,3' diol. A semiempirical study*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN II TRANSACTIONS, 1141-1147 (1995).
- [95-11] V.Barone, R.Fournier, F.Mele, N.Russo,C.Adamo, *Structure and EPR Parameters of CuC₂H₂ from a Density Functional Approach*, CHEMICAL PHYSICS LETTERS, **237**, 189-194 (1995).
- [95-12] E.Vauthier, M.Blain, S.Odiot,V.Barone, M.Comeau, S.Fliszár, *Xα Local spin Density Energy Calculations*, THEOCHEM, **340**, 63-71 (1995).
- [95-13] V.Barone, *Structure, Thermochemistry, and Magnetic Properties of Binary Copper Carbonyls by a Density-Functional Approach*, JOURNAL OF PHYSICAL CHEMISTRY, **99**, 11659-11666 (1995).
- [95-14] V.Barone, *Structure, Magnetic Properties and Reactivity of Open-Shell Species from Density Functional and Self-Consistent Hybrid Methods*, in Recent Advances in Density Functional Methods (Part I), edited by D.P.Chong, World Scientific Publishing Co. (1995), chapter 8, pages 287-334.
- [95-15] V.Barone, C.Adamo, *A Theoretical Study of Proton Transfer in [2,2'-bipyridyl]-3,3'diol*, CHEMICAL PHYSICS LETTERS, **241**, 1-6 (1995).
- [95-16] V.Barone, A.Bencini, F.Totti, M.G.Uytterhoeven, *A Theoretical Study of the Electronic Structure and of the Mercury-Carbon Bonding in Methyl-Mercury(II) Compounds*, JOURNAL OF PHYSICAL CHEMISTRY, **99**,12743-12750 (1995).
- [95-17] V.Barone,C.Adamo,A.Grand,R.Subra, *Structure and ESR Features of Glycine Radical in its Zwitterionic Form*, CHEMICAL PHYSICS LETTERS, **242**, 351-354 (1995).
- [95-18] V.Barone, L.Orlandini, C.Adamo, *Proton Transfer in Small Model Systems. A Density Functional Study*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **56**, 697-705 (1995).
- [95-19] V.Barone, C.Adamo, *Density Functional Study of Intrinsic and Environmental Effects in the Tautomer Equilibrium of 2-Pyridone*, JOURNAL OF PHYSICAL CHEMISTRY, **99**, 15062-15068 (1995).
- [95-20] N.Desmarais, C.Adamo, B.Panunzi, V.Barone, B.Giovannitti, *Origin and Fine Tuning of the Stability of Five-Coordinated Platinum (II) and Palladium (II) Species*, INORGANICA CHIMICA ACTA, **238**,159-163 (1995).
- [95-21] V.Barone, L.Orlandini, *Methyl Addition to Acetylene and Ethylene from a Density Functional Approach*, CHEMICAL PHYSICS LETTERS, **246**, 45-52 (1995).
- [95-22] V.Barone, C.Adamo, A.Grand, R.Subra, *ESR Features of the Bicyclobutyl Radical Revisited. A Counterintuitive Ordering of Short- and Long-Range Isotropic Hyperfine Coupling Constants*, CHEMICAL PHYSICS LETTERS, **246**, 53-58 (1995).

[95-23] V.Barone,C.Adamo,A.Grand,F.Jolibois,Y.Brunel,R.Subra, *Structure and ESR Features of Glycine Radical from Post Hartree-Fock Computations*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **117**, 12618-12624 (1995).

1994

[94-1] A.Zheludev, V.Barone, M.Bonnet, B.Delley, A.Grand, E.Ressouche, P.Rey, R. Subra, J.Schweizer, *Spin Density in a Nitronyl Nitroxide Free Radical. A Polarized Neutron Diffraction Investigation and Ab Initio Calculations*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, **116**, 2019-2027 (1994).

[94-2] V.Barone,C.Adamo, *Modulation of Intramolecular Proton Transfer by Electron Excitation and Environment. 2-Pyridone as a Case Study*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **15**, 395-404 (1994).

[94-3] V.Barone,C.Adamo,S.Fliszár, N.Russo, *Structural and Energetic Characteristics of Electron Deficient M_2H_6 Compounds from a Density Functional Approach*, CHEMICAL PHYSICS LETTERS, **222**, 597-602 (1994).

[94-4] R.Arnaud, H.Postlethwaite, V.Barone, *Theoretical Study of the Addition of tert-Butyl and Benzyl Radicals to Ethene*, JOURNAL OF PHYSICAL CHEMISTRY, **98**, 5913-5919 (1994).

[94-5] V.Barone,C.Adamo, *Proton Transfer in Excited Electronic States. Environmental Effects on the Tautomerization of 2-Pyridone*, JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY, SECTION A: CHEMISTRY, **80**, 211-219 (1994).

[94-6] C.Minichino, V.Barone, *From Concepts to Algorithms for the Characterization of Reaction Mechanisms. H_2CS as a Case Study*, JOURNAL OF CHEMICAL PHYSICS, **100**, 3717-3741 (1994).

[94-7] V.Barone,C.Adamo,N.Russo, *Density Functional Theory: an Effective Theoretical Tool for the Study of σ Radicals*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **52**, 963-971 (1994).

[94-8] C.Adamo, V.Barone, A.Fortunelli, *Density Functional Calculations of Isotopic Hyperfine Coupling Constants in β -ketoenyl Radicals*, JOURNAL OF PHYSICAL CHEMISTRY, **98**, 8648-8652 (1994).

[94-9] V.Barone, C.Adamo, *Theoretical Study of Direct and Water Assisted Isomerization of Formaldehyde Radical Cation. A Comparison between Density Functional and post Hartree-Fock Approaches*, CHEMICAL PHYSICS LETTERS, **224**, 432-438 (1994), erratum CHEMICAL PHYSICS LETTERS **228**, 499 (1994).

[94-10] V.Barone, *Inclusion of Hartree-Fock Exchange in the Density Functional Approach. Benchmark Computations for Diatomic Molecules Containing H, B, C, N, O, and F atoms*, CHEMICAL PHYSICS LETTERS, **226**, 392-398 (1994).

[94-11] V.Barone,C.Adamo, *A Theoretical Investigation of Potential Energy Surfaces Governing the Photochemical Tautomerization of 2-Pyridone*, CHEMICAL PHYSICS LETTERS **226**, 399-404 (1994).

[94-12] V.Barone, *Inclusion of Hartree-Fock Exchange in Density Functional Methods. Hyperfine Structure of Second Row Atoms and Hydrides*, JOURNAL OF CHEMICAL PHYSICS, **101**, 6834-6838 (1994).

[94-13] V.Barone, *Characterization of the Potential Energy Surface of the HO₂ Molecular System by a Density Functional Approach*, JOURNAL OF CHEMICAL PHYSICS, **101**, 10666-10676 (1994).

[94-14] V.Barone, L.Orlandini, C.Adamo, *Proton Transfer in Model Hydrogen-Bonded Systems by a Density Functional Approach*, CHEMICAL PHYSICS LETTERS, **231**, 295-300 (1994).

[94-15] F.Lelj, C.Adamo, V.Barone, *Role of Hartree-Fock Exchange in Density Functional Theory. Some Aspects of the Conformational Potential Energy Surface of Glycine in the Gas Phase*, CHEMICAL PHYSICS LETTERS, **230**, 189-195 (1994).

[94-16] V.Barone, L.Orlandini, C.Adamo, *Density Functional Study of Diborane, Dialane, and Digallane*, JOURNAL OF PHYSICAL CHEMISTRY, **98**, 13185-13188 (1994).

1993

[93-1] V.Barone, C.Minichino, H.Faucher, R.Subra, A.Grand, *Theoretical Investigation of the EPR Spectrum of the Cyclopropyl Radical*, CHEMICAL PHYSICS LETTERS **205**, 324-330 (1993).

[93-2] C.Adamo,V.Barone,S.Loison,C.Minichino, *Protomeric Equilibria in the Ground and Excited States of 2-Pyridone. A Semiempirical Study Including Solvent Effects*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANSACTIONS II, 697-702 (1993).

[93-3] V.Barone, A.Grand,C.Minichino,R.Subra, *A Theoretical Approach to the Structure and Hyperfine Coupling Constants of non Rigid Radicals. The Case of H₂NO*, JOURNAL OF PHYSICAL CHEMISTRY, **97**, 6355-6361 (1993).

[93-4] V.Barone,C.Adamo,N.Russo, *Density Functional Approach to the Structures and EPR Parameters of Open Shell Systems. The Case of Fluorovinyl Radicals*, CHEMICAL PHYSICS LETTERS, **212**, 5-11 (1993).

[93-5] V.Barone, A.Grand, D.Luneau, P.Rey, C.Minichino, R.Subra, *Ab-Initio Configuration Interaction Calculation of the Isotropic Spin Densities in Nitronyl- and Imino- Nitroxides*, NEW JOURNAL OF CHEMISTRY **17**,1587-1591 (1993).

[93-6] V.Barone,A.Grand,C.Minichino,R.Subra, *Vibrational Modulation Effects on the Hyperfine Coupling Constants of Fluoromethyl Radicals*, JOURNAL OF CHEMICAL PHYSICS, **99**, 6745-6756 (1993).

[93-7] C.Adamo,V.Barone, *Intrinsic and Environmental Effects on Protomeric Equilibria in the Ground and Excited Electronic States of Biological Systems*, in Chemistry and Properties of Biomolecular Systems, edited by N.Russo, J.Anastassopoulou, G.Barone, Kluwer (1993),1-18.

[93-8] R.Caputo,M.De Nisco,G.Palumbo,C.Adamo,V.Barone, *Chemistry of Ethanediyl S,S-Acetals 6. An Example of Vicarious Nucleophilic Substitution of Hydrogen in 1,4-Benzodithians*, TETRAHEDRON, **49**, 11383-1138 (1993).

[93-9] V.Barone,P.L.Cristinziano, *Theoretical Investigation of the Torsional Potential of 2,2'-Bipyrimidine*, CHEMICAL PHYSICS LETTERS, **215**, 40-44 (1993).

1992

[92-1] V.Barone,P.Jensen,C.Minichino, *Vibro-rotational Analysis of Si₂C from an Ab-initio Potential Energy Surface. A Comparison between Perturbative and Variational Methods*, JOURNAL OF MOLECULAR SPECTROSCOPY, **154**, 252-264 (1992).

[92-2] P.Amodeo, V.Barone, *A New General Form of Molecular Force Fields. Application to Intra- and Inter- Residue Interactions in Peptides*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **114**, 9085-9093 (1992).

1991

[91-1] C.Toniolo, M.Crisma, G.Valle, G.M.Bonora, F.Lelj, V.Barone, F.Fraternali, P.M.Hardy, H.L.S.Maia, *Conformational Analysis of Peptides from C^{α,α}-Symmetrically Disubstituted Aromatic α-Aminoacid Residues*, PEPTIDES 1990, E.Giralt, Ed., Escom, Leiden (1991).

[91-2] M.Crisma, G.Valle, G.M.Bonora, C.Toniolo,F.Lelj,V.Barone,F.Fraternali,P.M.Hardy, H.L.S. Maia, *Preferred Conformation of Peptides from C^{α,α}-Symmetrically Disubstituted Glycines: Aromatic Residues*, BIOPOLYMERS **31**, 637-641 (1991).

[91-3] V.Barone, C.Cauletti, M.N.Piancastelli, M.Ghedini, M.Toscano, *Acceptor Capacity and Donor Strength of Biphenyl-like α-Diimine Ligands. A Theoretical and Gas-Phase UV Photoelectron Spectroscopic Study*, JOURNAL OF PHYSICAL CHEMISTRY, **95**, 7217-7220 (1991).

[91-4] A.Grand, P.Rey, R.Subra, V.Barone, C.Minichino, *Ab-initio Study of Nitronyl- and Imino-Nitroxides. Relation Between Electronic Structure and Magnetic Properties in Metal-Nitroxide Complexes*, JOURNAL OF PHYSICAL CHEMISTRY, **95**, 9238-9242 (1991).

1990

[90-1] V.Barone, C.Minichino, N.Russo, M.Toscano, F.Illas, J.Rubio, *Non Empirical Cluster Model Study of the Relaxation of (111) Surfaces of C, Si, Ge*, THEOCHEM, **204**, 325-329 (1990).

[90-2] V.Barone,F.Fraternali,P.L.Cristinziano, *Sensitivity of Peptide Conformations to Methods and Geometrical Parameters. A Comparative Ab-Initio and Molecular Mechanics Study of α-Aminoisobutyric Acid*, MACROMOLECULES, **23**, 2038-2044 (1990).

[90-3] P.Amodeo, V.Barone, F.Fraternali, *Status and Perspectives of the Microscopic Approach to Structure and Thermodynamic Properties of Peptides and Proteins*, THERMOCHIMICA ACTA, **162**, 141-154 (1990).

[90-4] E.C.Vauthier, V.Barone, C.Minichino, S.Fliszár, *Xα Local Spin Density Calculations of 1:1 Hydrogen Bonded Complexes Formed by Water, Ammonia, and Hydrogen Fluoride*, CANADIAN JOURNAL OF CHEMISTRY, **68**, 1233-1237 (1990).

[90-5] M.Crisma, G.Valle, G.M.Bonora, E.De Menego, C.Toniolo, F.Lelj,V.Barone, F.Fraternali, *Structural Versatility of Peptides from C^{α,α}-Disubstituted Glycines. Preferred Conformation of the C^{α,α}-Diphenylglycine Residue*, BIOPOLYMERS, **30**, 1-11 (1990).

[90-6] C. Toniolo, G. Valle, M. Crisma, G.M.Bonora, F.Lelj, P.L.Cristinziano, V.Barone, D. Nisato, *Theoretical and Experimental Conformational Analysis of two Diastereoisomeric "Val"-Statine Derivatives*, PEPTIDE RESEARCH, **3**, 27-34 (1990).

[90-7] G. Valle, M.Crisma, G.M.Bonora, C.Toniolo, F.Lelj, V.Barone, F.Fraternali, P.M. Hardy, A. Langran-Goldsmith, H.L.S.Maia, *Structural Versatility of Peptides from C^{α,α}-Disubstituted Glycines. Preferred Conformation of C^{α,α}-Dibenzylglycine Residue*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN II TRANS., 1481-1487 (1990).

1989

[89-1] P.L.Cristinziano, F.Lelj, P.Amodeo, G.Barone, V.Barone, *Stability and Structure of Formamide and Urea Dimers in Aqueous Solution. A Theoretical Study*, JOURNAL OF THE CHEMICAL SOCIETY, FARADAY TRANS. I, **85**, 621-632 (1989).

[89-2] V.Barone, C.Minichino, *A theoretical characterization of the structure formation enthalpy, and fluzional behaviour of B₂H₆ and AlBH₆*, THEORETICA CHIMICA ACTA, **76**, 53-64 (1989).

[89-3] V.Barone, N.Russo, M.Toscano, *Interaction of Atomic Hydrogen with the (111) and (100) Surfaces of Diamond-like Crystals*, in "Structure and Reactivity of Surfaces", ed. C.Morterra, A.Zecchina, G.Costa, Elsevier Science Publishers B.V.,Amsterdam, 69-73 (1989).

[89-4] M.Crisma, G.M.Bonora, C.Toniolo, V.Barone, E.Benedetti, B.Di Blasio, V.Pavone, C. Pedone, A.Santini, F.Fraternali, A.Bavoso, F.Lelj, *Structural Versatility of Peptides Containing C^{α,α}-dialkylated Glycines. Conformational Energy Computations, Infrared Absorption and ¹H nmr analysis of 1-Aminocyclopropane-1-carboxylic Acid Homopeptides*, INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES, **11**, 345-352 (1989).

[89-5] E.Benedetti, B.Di Blasio, V.Pavone, C.Pedone, A.Santini,V.Barone, F.Fraternali, F.Lelj, A.Bavoso, M.Crisma, C.Toniolo, *Structural Versatility of Peptides Containing C^{α,α}-Dialkyated Glycines. An X-ray Diffraction Study of Six 1-Amino Cyclopropane-1-Carboxylic Acid Rich Peptides*, INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES, **11**, 353-360 (1989).

1988

[88-1] E.Benedetti, V.Barone, A.Bavoso, B.Di Blasio, F.Lelj, V.Pavone,C.Pedone, G.M. Bonora, C. Toniolo,M.T.Leplawy,K.Kaczmarek, A.Redlinski, *Structural Versatility of Peptides from Ca,a-Dialkylated Glycines. I. A Conformational energy Computation and X-Ray Diffraction Study of Homo-Peptides from C^{α,α}-Diethylglycine*, BIOPOLYMERS, **27**, 357-371 (1988).

[88-2] C.Toniolo, G.M.Bonora, A.Bavoso, E.Benedetti, B.Di Blasio, V.Pavone, C.Pedone, V.Barone, F.Lelj, M.T.Leplawy, K.Kaczmarek, A.Redlinski, *Structural Versatility of Peptides from C^{α,α}-Dialkylated Glycines. II. An IR Adsorption and 1H NMR Study of Homo-Oligopeptides from C C^{α,α}-Diethylglycine*, BIOPOLYMERS, **27**, 373-379 (1988).

[88-3] N.Russo, M.Toscano, P.Amodeo, V.Barone, *Non Empirical Cluster Model Study of the Chemisorption of Fluorine and Chlorine on the (111) Surface of Diamond*, SOLID STATE COMMUNICATIONS, **65**, 935-937 (1988).

[88-4] V.Barone, C.Minichino, N.Russo, M.Toscano, *Model Clusters and Electronic Characteristics of Deep Level Impurities in Silicon*, PHYSICA STATUS SOLIDI, **145**, k125-130 (1988).

[88-5] V.Barone, *Modelli e metodi teorici per lo studio del meccanismo di reazioni chimiche*, in "Equilibri in soluzione:aspetti teorici, sperimentali ed applicativi" a cura di C.La Mesa, A.Napoli, N.Russo e M.Toscano, Marra Editrice (Cosenza, 1988) 196-218.

[88-6] V.Barone, C.Minichino, F.Lelj, N.Russo, *Ab-Initio Pseudopotential Study of the Fluxional behaviour in Tetrahydroborate Complexes. Many-Body Contributions to the energy Barriers of NaBH₄ and AlH₂BH₄*, JOURNAL OF COMPUTATIONAL CHEMISTRY, **9**, 518-521(1988).

[88-7] V.Barone, G.Del Re, C.Barbier, G.Villani, *A priori Hybridisation with the Maximum Localisation Criterium. General Aspects and New Developments*, GAZZETTA CHIMICA ITALIANA, **118**, 347-358 (1988).

[88-8] C.Toniolo, M.Crisma, G. Valle, G.M.Bonora, V. Barone, E. Benedetti, B.Di Blasio, V.Pavone, C. Pedone, A.Santini, F.Lelj, *Structural Versatility of Peptides from C^{α,α}-Dialkylated Glycines: Acc3-Rich Peptides*, PEPTIDE CHEMISTRY 87, Ed.T.Shiba & S.Sakakibara, Protein Research Foundation, Osaka, 1988, pp.45-48.

[88-9] V.Barone, C.Minichino, S.Fliszár, N.Russo, *Structural and Electronic Origin of the Conformational Behaviour of Biphenyl-like α-Diimine Ligands. A Theoretical Study*, CANADIAN JOURNAL OF CHEMISTRY, **66**, 1313-1317 (1988).

[88-10] V.Pavone, E.Benedetti, V.Barone, B.Di Blasio, F.Lelj, C.Pedone, A.Santini, M.Crisma, G.M.Bonora, C.Toniolo, *Structural Versatility of Peptides from C^{α,α}-Dialkylated Glycines. A Conformational energy Computation and X-Ray Diffraction Study of Homo-peptides from 1-Amino-Cyclohexane-1-Carboxylic Acid*, MACROMOLECULES **21**, 2064-2071 (1988).

[88-11] V.Barone, C.Minichino, N.Russo, M.Toscano, *Conformational Behaviour of Nonfused Biheterocycles. The case of Isomeric PhenylFurans*, GAZZETTA CHIMICA ITALIANA, **118**, 753-756 (1988).

[88-12] V.Barone, F.Frernali, P.L. Cristinziano, F.Lelj, A.Rosa, *Conformational Behaviour of C^{α,α}-Dialkylated Peptides. Ab-Initio and Empirical Computations for Cyclo-propylglycine*, BIOPOLYMERS, **27**, 1673-1685 (1988).

[88-13] A.Santini, V.Barone, A.Bavoso, E.Benedetti, B.Di Blasio, F.Frernali, F.Lelj, V. Pavone, C.Pedone, M.Crisma, G.M.Bonora, C.Toniolo, *Structural Versatility of Peptides from C^{α,α}-Dialkylated Glycines. A Conformational energy Computation and X-Ray Diffraction Study of Homo-peptides from 1-Amino-Ciclopentane-1-Carboxylic Acid*, INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES, **10**, 292-299 (1988).

[88-14] V.Barone, F.Lelj, C.Minichino, N.Russo, M.Toscano, *Conformational Behaviour of Nonfused Biheterocycles. Part XI. 2,2'-Bi-imidazolyl*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN II TRANS., 1975-1977(1988).

[88-15] N.Russo, M.Toscano, V.Barone, *Conformational Behaviour of Nonfused Bihe-terocycles. Part X. Isomeric Phenylisoxazoles*, JOURNAL OF HETEROCYCLIC CHEMISTRY, **25**, 1709-1712 (1988).

[88-16] N.Russo,P.Grande,M.Toscano,V. Barone, *Structure and Relative Stabilities of $C_3H_8N^+$ Ions: a Theoretical Study*, ADVANCES IN MASS SPECTROMETRY **11A**, 946-947 (1988).

1987

[87-1] N.Russo, M.Toscano, V.Barone, F.Lelj, *On the Chemisorption of Water on the (100) Surface of Silicon*, SURFACE SCIENCE, **180**, 599-604 (1987).

[87-2] V.Barone, F.Lelj, P.Grande, N.Russo, M.Toscano, *The Fragmentation of $C_2H_6N^+$ Ions. An Alternative Mechanism*, CHEMICAL PHYSICS LETTERS, **133**, 548-555 (1987).

[87-3] E. Iaconis, N. Russo, M. Toscano, V. Barone, C. Minichino, *Interaction of Carbon Atom with the Basal Plane of Graphite. A Theoretical Study*, GAZZETTA CHIMICA ITALIANA, **117**, 57-59 (1987).

[87-4] N.Russo, R.Subra, M.Toscano, V.Barone, *The Structure of the Ammonia-Boryl Radical (BH_2NH_3), an Inorganic Analogue of the Ethyl Radical. A Non-Empirical Study*, THEOCHEM, **36**, 365-371 (1987).

[87-5] N.Russo, M.Toscano, V.Barone, C.Minichino, *Conformational Behaviour of Aromatic Systems. Part 10. Isomeric Phenylpyrroles*, JOURNAL DE CHIMIE PHYSIQUE, **84**, 735-738 (1987).

[87-6] V.Barone, F.Lelj, N.Russo, M.Toscano, *Adsorption of H_2O and H_2S on the (100) Surface of Silicon. A Theoretical Study*, JOURNAL DE CHIMIE PHYSIQUE, **84**, 799-803 (1987).

[87-7] P.L.Cristinziano, F.Lelj, P.Amodeo, V.Barone, *A Molecular Dynamics Study of Molecular Associations in Solution. An NPT Simulation of Urea Dimer in Water*, CHEMICAL PHYSICS LETTERS, **140**, 401-405 (1987).

[87-8] E.Benedetti, V.Barone, A.Bavoso, B.Di Blasio, F.Lelj, V. Pavone, C.Pedone, C. Toniolo, M.Crisma, G.M.Bonora, *Structural Versatility of Peptides from α,α -Dialkylated Glycines: Acc5- and Acc6- Containing Peptides*, PEPTIDES 1986, Ed.D.Theodoropoulos, Walter de Gruyter & Co., 1987, pp.315-318.

[87-9] C.Toniolo, G.Valle, G.M.Bonora, F.Lelj, V.Barone, F.Frernali, G.Callet, J.Wagnon, D.Nisato, *Conformational Preferences and Self-Association Modes of Two Diastereomeric Statine Derivatives*, INTERNATIONAL JOURNAL OF PEPTIDES AND PROTEIN RESEARCH **30**, 583-595 (1987).

[87-10] V.Barone, *The Cluster Approach in the Study of Atomic and Molecular Chemisorption on Silicon*, SURFACE SCIENCE, **189**, 106-113 (1987).

[87-11] V.Barone, F.Lelj, C.Minichino, N.Russo, M.Toscano, *Cluster-Model Study of the Chemisorption of Atomic Hydrogen on the Basal Plane of Graphite*, SURFACE SCIENCE, **189**, 185-189 (1987).

[87-12] V.Barone, *Costruzione di superfici di potenziale per biomolecole e loro composti modello tramite calcoli di meccanica molecolare*, Seminario Nazionale di Chimica-Fisica 1987, a cura di G.Barone.

1986

[86-1] R.Barbucci, M.Casolaro,M.Nocentini, S.Corezzi, P.Ferruti, V.Barone, *Acid-Base and Metal Ion Complex Formation Properties of Polymers Containing Amino-Acid residues*, MACROMOLECULES, **19**, 37-42 (1986).

[86-2] V.Barone, F.Lelj, E.Iaconis, F.Illas, N.Russo, A.Jonnou, *Quantum-mechanical study of the Chemisorption of Atomic and Molecular Oxygen on Graphite Clusters*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM), **29**, 313-322 (1986).

[86-3] V.Barone, F.Lelj, N.Russo, M.Toscano, *Conformational Behaviour of Isomeric Bi-thienyls. An ab-initio Study*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANS. 2, 907-910 (1986).

[86-4] V.Barone, F.Lelj, N.Russo, *Conformational Behaviour of Azabiphenyls*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, **29**, 541-551 (1986).

[86-5] R.Arnaud, R.Subra, V.Barone, F.Lelj, S.Olivella, A.Solé, N.Russo, *Ab-Initio Mechanistic Studies of Radical Reactions.Directive effects in the Addition of Methyl Radical to unsymmetrical Fluoroethenes*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANS. 2, 1517-1524 (1986).

[86-6] V.Barone, F.Lelj, N.Russo, M.Toscano, *On the Interaction of Halogen Atoms with (111) and (100) Surfaces of Silicon*, SOLID STATE COMMUNICATIONS, **59**, 433-436 (1986).

[86-7] V.Barone, F.Lelj, E.Iaconis, F.Illas, N.Russo, *A Theoretical Study of the Nitrogen-Graphite System*, THEOCHEM, **32**, 277-282 (1986).

[86-8] V.Barone, F.Lelj, N.Russo, M.Toscano, F.Illas, J.Rubio, *Non-Empirical Cluster Model Study of the Chemisorption of Atomic Hydrogen on the (111) Surface of Diamond-Like Crystals*, PHYSICAL REVIEW B, **34**, 7203-7208, (1986).

[86-9] R.Barbucci, M.Casolaro, M.Nocentini, V.Barone, P.Ferruti, *Coordination Chemistry of Metal Ions with Macromolecular Ligands,in Metal Complexes in Solution*, a cura di E.A.Jenne, E. Rizzarelli, V.Romano, S.Sammartano, Piccin Nuova Libreria SPA, Padova, 133-154 (1986).

1985

[85-1] G.Abbate, V.Barone, F.Lelj, E.Iaconis, N.Russo, *Model Hamiltonians in the Study of Chemisorption and Catalysis*, SURFACE SCIENCE **152**, 690-701 (1985).

[85-2] C. Toniolo, G.M. Bonora, V. Barone, A. Bavoso, E. Benedetti, B. Di Blasio, P. Grimaldi, F. Lelj, V. Pavone, C. Pedone, *Conformation of Pleionomers of α -Aminoisobutyric Acid*, MACROMOLECULES **18**, 895-902 (1985).

[85-3] V.Barone, L.Commisso, F.Lelj, N.Russo, *Conformational Behaviour of Phenylpyrimidines. A Non Empirical Quantum Mechanical Study*, TETRAHEDRON **41**, 1915-1918 (1985).

- [85-4] V.Barone, F.Lelj, L.Commisso, N.Russo, C.Cauletti,M.N.Piancastelli, *Experimental and Theoretical Approach to the Electronic Structure and the Molecular Conformation of Azabiphenyls. Asymmetric Bipyridines*, CHEMICAL PHYSICS **96**, 435-445 (1985).
- [85-5] C.Toniolo, G.M.Bonora, V.Barone, A.Bavoso, E.Benedetti, B.Di Blasio, F.Lelj, V. Pavone, C.Pedone, *α -Methyl, α -Amino Acids in Peptide Chemistry: Conformation of Pleionomers of α -Aminoisobutyric Acid*, INTERNATIONAL FORUM ON PEPTIDES, B.Castro, J. Martinez, Eds., Hermann Paris,1985.
- [85-6] R.Arnaud, V.Barone, S.Olivella, A.Solé, *Ab-Initio Mechanistic Studies of Radical Reactions. Addition of Methyl Radicals to Acetylene and Ethylene*, CHEMICAL PHYSICS LETTERS **118**, 573-579 (1985).
- [85-7] V.Barone, A.Gavezzotti, N.Russo e M.Simonetta, *Superfici e Chemisorbimento. Calcoli Teorici con il Modello degli Aggregati*, in "Problemi e Metodi di Scienza delle Superfici",a cura di G.Del Re pp.23-43 (1985).
- [85-8] R.Arnaud, V.Barone, S.Olivella, N.Russo, A.Solé, *Theoretical Study of Regioselectivity in Methyl Radical Additions to Fluoroethenes*, JOURNAL OF THE CHEMICAL SOCIETY (CHEMICAL COMMUNICATIONS),1331-1332 (1985).
- [85-9] V.Barone, F.Lelj, G.Abbate, *Fractional Populations of Individual Conformers in Multidihedral Systems. A J coupling Constant Approach*, MAGNETIC RESONANCE IN CHEMISTRY **23**, 715-719 (1985).
- [85-10] V.Barone, F.Lelj, A.Bavoso,B.Di Blasio, P.Grimaldi, V.Pavone, C.Pedone, *Conformational Behaviour of α,α -Dialkylated Peptides*, BIOPOLYMERS **24**, 1759-1767 (1985).
- [85-11] R. Arnaud, S. Choubani, R. Subra, M. Vidal, M. Vincens, V. Barone, *Le Radical Methylenecyclopropyle: Etude theorique, Chloration par tBuOCl et Reduction par (nBu)₃SnH de Derives Cyclopropeniques*, CANADIAN JOURNAL OF CHEMISTRY **63**, 2512-2521 (1985).
- [85-12] V.Barone, F.Lelj, P.Grande, N.Russo, *Structures and Relative Stabilities of [C₂H₆N]⁺ Ions. A non empirical and MNDO Study*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM), **25**, 319-324 (1985).
- [85-13] N.Russo, M.Toscano, V.Barone, F.Lelj, *Chemisorption of Atomic and Molecular Oxygen on the (100) Surface of Silicon. A Theoretical Study*, SURFACE SCIENCE, **162**, 230-238 (1985).
- [85-14] V.Barone, F.Lelj, N.Russo, M.Toscano, F.Illas, J.Rubio, *A Theoretical Study of Relaxation and Reconstruction of the (111) Surface of Diamond*, SURFACE SCIENCE, **162**, 169-174 (1985).
- [85-15] N.Russo, M.Toscano, V.Barone, F.Lelj, *Theoretical Study of Oxygen Chemisorption on (111) and (100) Silicon Surfaces*, PHYSICS LETTERS, **113A**, 321-324 (1985).

[84-1] V.Barone, N.Bianchi, F.Lelj, N.Russo, G.Abbate, *A Non-Empirical and HAM/3 Study of Geometry, Conformational Behaviour and Electronic Structure of Isomeric Vinylpyridines*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **17**, 35-43 (1984).

[84-2] V.Barone, F.Lelj, N.Russo, G.Abbate, *Surface Relaxation and Reconstruction in Diamond-Like Crystals*, SOLID STATE COMMUNICATIONS **49**, 925-928 (1984).

[84-3] M.C.Tanzi, L.Rusconi, C.Barozzi, P.Ferruti, L.Angiolini, M. Nocentini, V.Barone, R.Barbucci, *Synthesis and Characterization of Piperazine-Derived Poly(Amido-Amine)s with Different Distributions of Amido- and Amino-Groups Along the Macromolecular Chain*, POLYMER **25**, 863-868 (1984).

[84-4] V.Barone, F.Lelj, O.Nicolaus, G.Abbate, R.Barbucci, *The Mechanism of Protonation of Diamines in Aqueous Solution: a ¹³C NMR Investigation*, GAZZETTA CHIMICA ITALIANA **114**, 249-251 (1984).

[84-5] G.Del Re, V.Barone, F.Lelj, *The Mechanisms of Elementary Physico-Chemical Processes: an Introductory Report*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **26**, 563-591 (1984).

[84-6] V.Barone, C.Cauletti, L.Commisso, F.Lelj, M.N.Piancastelli, N.Russo, *Quantum-Chemical and UV Photoelectron Spectroscopic Studies of AzaBiphenyls. The Case of 4-Phenylpyridine*, JOURNAL OF CHEMICAL RESEARCH S 338-339 (1984).

[84-7] V.Barone, N.Bianchi, F.Lelj, N.Russo, *Gas Phase Unimolecular 1,1 Hydrogen Elimination: Reaction Mechanism and Isotope Effect*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **26**, 621-636 (1984).

[84-8] P.Corradi, G.Guerra, V.Barone, *Conformational Analysis of Polypropylene Chains Bound to Model Catalytic Sites*, EUROPEAN POLYMER JOURNAL **20**, 1177-1182 (1984).

[84-9] N.Montella, V.Barone, G.Del Re, *Charge-Transfer in Adsorbate-Substrate Systems. Extension of the Anderson-Newns Treatment to Two- and Three-Dimensional Substrates*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **26**, 769-774 (1984).

[84-10] E.Benedetti, C.Toniolo, P.Hardy, V.Barone, A.Bavoso, B.Di Blasio, P.Grimaldi, F.Lelj, V.Pavone, C.Pedone, G.M.Bonora, I.Lingham, *Folded and Extended Structures of Homo-Oligopeptides from α,α -Dialkylated Aminoacids. A Conformational Energy Computation and X-Ray Diffraction Study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **106**, 8146-8152 (1984).

[84-11] E.Benedetti, V.Barone, A.Bavoso, B.Di Blasio, P.Grimaldi, F.Lelj, V.Pavone, C.Pedone, G.M. Bonora,C.Toniolo, I.Lingham, P.M.Hardy, *Folded and Extended Structures of Homo-Peptides from α,α -Dialkylated α -Amino Acids*, PEPTIDES 84, Ragnarsson, Ahquist, Wiksell, Eds., International, Stockholm, Sweden (1984), pp.603-606.

1983

[83-1] R.Barbucci, M.Casolaro, V.Barone, P.Ferruti, A.Angeloni, *Effect of Different Shielding Groups on the Polyelectrolyte Behaviour of Polyamines*, MACROMOLECULES **16**, 456-462 (1983).

[83-2] R.Barbucci, M.Casolaro, V.Barone, P.Ferruti, M.Tramontini, *Macroinorganics 9. Enthalpies of Protonation and Complex Formation with Copper (II) Ion of some Poly(Amido-Amine)s*, MACROMOLECULES **16**, 1159-1164 (1983).

[83-3] V.Barone, P.L.Cristinziano, F.Lelj, A.Pastore, N.Russo, *Nonempirical Analysis of Unusual Chemical Bonds. Part III:[LiBH(NH₂)]⁺*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **9**, 103-108 (1983).

[83-4] V.Barone, F.Lelj, N.Russo, Y.Ellinger, R.Subra, *Theoretical Approach to Fluorine Substitution in X₂NO and X₂CN Free Radicals. Comparison Between Ab-Initio UHF and RHF + Perturbation Treatments*, CHEMICAL PHYSICS **76**, 385-396 (1983).

[83-5] V.Barone, F.Lelj, C.Cauletti, M.N.Piancastelli, N.Russo, *General Trends in the Molecular Physics of Azabiphenyls. A Quantum Chemical and Photoelectron Spectroscopic Study*, MOLECULAR PHYSICS **49**, 599-619 (1983).

[83-6] V.Barone, G.Del Re, *Hybridization and Surface Relaxation in Diamond-Like Clusters*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **11**, 173-185 (1983).

[83-7] V.Barone, N.Bianchi, F.Lelj, *Transition State Structure and Isotope Effects in Unimolecular Hydrogen Elimination from Carbocations* CHEMICAL PHYSICS LETTERS **98**, 463-466 (1983).

[83-8] A.Bavoso, E.Benedetti, B.Di Blasio, V.Pavone, C.Pedone, V.Barone, G.Esposito, F.Lelj, G.P.Lorenzi, *Conformational Features of Alternating L,D Peptides*, PEPTIDES 1982, K.Blaha and P.Malon Eds., Walter de Gruyter Berlin-New York (1983) pp.699-704.

[83-9] V.Barone,G.Del Re, A.Lami, G.Abbate, *Bond Orbital Models II. Construction of Zero-Non-Bonding- Overlap Hybrids and their Use in Approximate Molecular Computations*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **14**, 191-200 (1983).

[83-10] P.Corradi, V.Barone, R.Fusco, G.Guerra, *A Possible Model of Catalytic Sites for the Stereospecific Polymerization of α-Olefins on First-Generation and Supported Ziegler-Natta Catalysts*, GAZZETTA CHIMICA ITALIANA **113**, 601-607 (1983).

[83-11] C.Pedone, V.Barone, E.Benedetti, B.Di Blasio, G.Esposito, F.Lelj, V.Pavone, G.P.Lorenzi, *Channel-Forming Molecules: Conformation of Peptides with Alternating L and D Residues as Models of Gramicidin A*, PEPTIDES: STRUCTURE AND FUNCTION; V.J. Hruby, D.H.Rich, Eds., Pierce Chemical Company, Rockford, Illinois (1983), pp.473- 476.

1982

[82-1] V.Barone, P.L.Cristinziano, F.Lelj, N.Russo, *Theoretical Studies on the Geometric and Electronic Structure of Substituted SCN Isomers I. Non-Empirical and MNDO Results for some Thiocyanates*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **3**, 239-253 (1982).

[82-2]R.Barbucci, M.Casolaro, P.Ferruti, V.Barone, *Macroinorganics VIII. Chelation of Copper (II) Ion with some New Poly(amido-amine)s*, POLYMER **23**, 148-151 (1982).

[82-3] R.Arnaud, R.Subra, V.Barone, *Substituent Effects and Radical Reactivity: Addition of p-Substituted Phenyl Radicals to Ethylene*, NOUVEAU JOURNAL DE CHIMIE **6**, 91-95 (1982).

[82-4] R.Barbucci, M.Casolaro, M.C.Beni, N.Danzo, V.Barone, P. Ferruti, *Thermodynamics of Protonation and Complex Formation of Multifunctional Polymers*, GAZZETTA CHIMICA ITALIANA **112**, 105-113 (1982).

[82-5] V.Barone, P.L.Cristinziano, F.Lelj, A.Pastore, N.Russo, *Conformational Effects and Lone Pair Levels of Diaza Compounds. 2,2'-Bipyridine and 4,5-Diazaphenanthrene as Test Cases*, GAZZETTA CHIMICA ITALIANA **112**, 195-198 (1982).

[82-6] V.Barone, C.Cauletti, F.Lelj, M.N.Piancastelli, N.Russo, *Relative Ordering and Spacing of n and π Levels in Isomeric Bipyrimidines. A Theoretical and Gas Phase UV Photoelectron Spectroscopic Study*, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY **104**, 4571-4578 (1982).

[82-7] V.Barone, P.L.Cristinziano, F.Lelj, A.Pastore, N.Russo, *Non Empirical and MNDO Study of the Geometry and Electronic Structure of H_2XO Radicals*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **7**, 59-64 (1982).

[82-8] P.Corradi, R.Fusco, V.Barone, F.Guerra, *Steric Control in Ziegler-Natta Catalysts: an Analysis of Non Bonded Interactions at Model Catalytic Sites*, JOURNAL OF CATALYSIS **77**, 32-42 (1982).

[82-9] P.Corradi, V.Barone, G.Guerra, *Steric Control in the First Step of the Isospecific Ziegler-Natta Polymerization of Propene*, MACROMOLECULES **15**, 1242-1245 (1982).

[82-10] F.Lelj, V.Barone, *Metodi Quantomeccanici e Chimica di Ioni in Fase Gassosa*, in INTRODUZIONE ALLA SPETTROMETRIA DI MASSA ORGANICA a cura di Nicola Uccella, Societa Chimica Italiana, Gruppo di Spettrometria di Massa (1982) pp 133-152.

[82-11] A.Laforgue, C.Brucena-Grimbert, D.Laforgue-Kantzer, G.Del Re, V. Barone, *Theoretical Analysis of Conduction in Acid and Base Solutions*, JOURNAL OF PHYSICAL CHEMISTRY **86**, 4436-4446 (1982).

1981

[81-1] V.Barone, P.Bucci, F.Lelj, N.Russo, *An Ab-initio Reinvestigation of the Geometric and Electronic Structure of Boron Trioxide*, JOURNAL OF MOLECULAR STRUCTURE (THEOCHEM) **1**, 29-35 (1981).

[81-2] P. Ferruti, N. Danzo, L.Oliva, R.Barbucci, V.Barone, *Macroinorganics. Part 6. Protonation and Complex Formation of a New Series of Polymers whose Repeating Units Behave Independently*, JOURNAL OF THE CHEMICAL SOCIETY, DALTON TRANS., 539-542 (1981).

[81-3] R.Barbucci, V.Barone, M.Micheloni, L.Rusconi, *Thermodynamics of Protonation of Tetramines with Different Degrees of N-Methylation*, JOURNAL OF PHYSICAL CHEMISTRY **85**, 64-68 (1981).

[81-4] R.Barbucci, V.Barone, P.Ferruti, L.Oliva, *Thermodynamics of Protonation of Polymeric Bases whose Repeating Units Behave Independently*, JOURNAL OF POLYMER SCIENCE, POLYMER SYMPOSIA **69**, 49-66 (1981).

[81-5] V.Barone, G.Dolcetti, F.Lelj, N.Russo, *Transition Metal Tetrahydroborate Complexes as Catalysts I: Non Empirical Determination of Static, Dynamic, and Chemical Properties of the Model Compounds NaBH₄ and AlH₂BH₄*, INORGANIC CHEMISTRY **20**, 1687-1691 (1981).

[81-6] V.Barone, F.Lelj, N.Russo, *Theoretical Conformational Analysis of Phosphonium-Acetylcholine and Arsonium-Acetylcholine*, GAZZETTA CHIMICA ITALIANA **111**, 75-79 (1981).

[81-7] V.Barone, R.Barbucci, N.Russo, *Intrinsic Basicities and Structural Modifications in the Stepwise Protonation of Aliphatic Amines*, GAZZETTA CHIMICA ITALIANA **111**, 115-121 (1981).

[81-8] V.Barone, F.Lelj, N.Russo, *Non-empirical Analysis of Unusual Chemical Bonds II. AlH₂BH₄ and AlH₂C₃H₅*, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **19**, 1197-1201 (1981).

[81-9] R.Barbucci, M.Casolaro, P.Ferruti, V.Barone, F.Lelj, L. Oliva, *Macroinorganics VII. Properties-Structure Relationships for Polymeric Bases whose Monomeric Units Behave Independently toward Protonation*, MACROMOLECULES **14**, 1203-1209 (1981).

1980

[80-1] J.Douady, V.Barone, Y.Ellinger, R.Subra, Perturbative Configuration Interaction Using Localized Orbitals in the INDO Hypothesis. I:Theory and Application to Energetic Problems, INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY **17**, 211-233 (1980).

[80-2] M.Delfini, A.L.Segre, F.Conti, R.Barbucci, V.Barone, P. Ferruti, *On the Mechanism of Protonation of Triamines*, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANS. 2, 900-903 (1980).

[80-3] R.Barbucci, V.Barone, P.Ferruti, M.Delfini, *Macroinorganics 3. The Chelation of Copper (II) Ion with Some Polymers Having a Poly(Amido-Amine) Structure and their non Macromolecular Models*, JOURNAL OF THE CHEMICAL SOCIETY, DALTON TRANS., 253-256 (1980).

[80-4] G.Del Re, V.Barone, N.Montella, A.Julg, *On the Shapes of Weakly Adsorbed Two Dimensional Clusters*, SURFACE SCIENCE **97**, 537-552 (1980).

[80-5] Y.Ellinger, F.Pauzat, V.Barone, J.Douady, R.Subra, Ab-Initio Study of the Vibrational Dependence of Hyperfine Coupling Constants in the Methyl, Silyl and Formaldehyde Anion Radicals, JOURNAL OF CHEMICAL PHYSICS **72**, 6390-6397 (1980).

[80-6] R.Barbucci, V.Barone, P.Ferruti, L.Oliva, T.Soldi, M.Pesavento, C.Bertoglio-Riolo, *Macro-Inorganics. Coordination Compounds with poly(amido-amine)s. "(IUPAC)"- Polymeric amines and ammonium salts*, Ed. E.J.Goethals, Pergamon Press, Oxford, N.Y., 263-269, 1980

[80-7] V.Barone, G.Del Re, G.Le Lay, R.Kern, Adsorption Sites and Relative Stabilities of the 3x1 and $\sqrt{3}$ Phases of Ag on Si(111), SURFACE SCIENCE **99**, 223-232 (1980).

[80-8] P.Corradi, G.Guerra, R.Fusco, V.Barone, *Analysis of Models for the Ziegler-Natta Stereospecific Polymerization on the Basis of Non-Bonded Interactions at the Catalytic Site 2. Edges*,

Steps and Reliefs on the Surfaces of Layered Modifications of TiCl₃, EUROPEAN POLYMER JOURNAL **16**, 835-842 (1980).

[80-9] V.Barone, F.Lelj, N.Russo, *Conformational Analysis of N-(\square -Acetoxyethyl) Pyridinium Ion: Comparison with Acetylcholine*, MOLECULAR PHARMACOLOGY **18**, 331-334 (1980).

[80.10] V.Barone, L.Oliva, R.Barbucci, *Theoretical Studies on the Protonation of Amines in Aqueous Solution*, INORGANICA CHIMICA ACTA **40**, X57-X58 (1980).

[80.11] L.Oliva, R.Barbucci, V.Barone, *Thermodynamic Studies on the Protonation and Complex-Formation of New Tertiary Amino Polymers in Aqueous Solution*, INORGANICA CHIMICA ACTA **40**, X58-X59 (1980).

1979

[79-1] J.Douady, V.Barone, Y.Ellinger, R.Subra, PCILINDO: the PCILO Method at the INDO Level, QUANTUM CHEMISTRY PROGRAM EXCHANGE **11**, 371 (1979).

[79-2] R.Barbucci, V.Barone, A Rationalization of the Enthalpy Values in the Protonation of Polyamines, JOURNAL OF SOLUTION CHEMISTRY **8**, 427-438 (1979).

[79-3] V.Barone, J.Douady, Y.Ellinger, R.Subra, F.Pauzat, Non-Empirical Calculations on the Conformation and Hyperfine Structure of the Silyl Radical. Influence of Vibrational Effects, CHEMICAL PHYSICS LETTERS **65**, 542-548 (1979).

[79-4] V.Barone, G.Del Re, S.Fliszár, Substituent Effects and the Strengths of Chemical Bonds, JOURNAL OF THE CHEMICAL SOCIETY, PERKIN TRANS. **2**, 1309-1316 (1979).

[79-5] V.Barone, J.Douady, Y.Ellinger, R.Subra, G.Del Re, Bond Orbital Models. Part 1: Atomic Charges from a Fully Localized SCF Method, JOURNAL OF THE CHEMICAL SOCIETY FARADAY TRANS. **2**, **75**, 1597-1611 (1979).

[79-6] P.Corradi, V.Barone, R.Fusco, G.Guerra, Analysis of Models for the Ziegler-Natta Stereospecific Polymerization on the Basis of Non-Bonded Interactions at the Catalytic Site. I: the Cossee Model, EUROPEAN POLYMER JOURNAL **15**, 1133-1141 (1979).

1978

[78-1] R.Barbucci, V.Barone, P.Ferruti, *Basicità e Capacità Complessanti di Poli(Ammido-Ammine) e loro Modelli non Macromolecolari in Soluzione Acquosa*, ATTI ACCADEMIA NAZIONALE DEI LINCEI **64**, 481-484 (1978).

1977

[77-1] A.Julg, G.Del Re, V.Barone, A Theoretical Study of Distortions Induced by Finite Size in Regular Clusters, PHYLOSOPHICAL MAGAZINE **35**, 517-535 (1977).

[77-2] A.Julg, G.Del Re, M.Bourg, V.Barone, Geometrical Relaxation of Model Metallic Clusters, JOURNAL DE PHYSIQUE **38**, 29-32 (1977).