ACCADEMIA NAZIONALE DEI LINCEI E FONDAZIONE «GUIDO DONEGANI»

QUANTUM CHEMISTRY AND CHEMINFORMATICS

26-27 SEPTEMBER 2024

ROME PALAZZO CORSINI - VIA DELLA LUNGARA, 10

A B S T R A C T

Comitato ordinatore: Vincenzo AQUILANTI (Linceo, Università di Perugia), Vincenzo BARONE (Linceo, Scuola Normale Superiore Pisa), Sergio CARRÀ (Linceo, Politecnico di Milano), Cecilia COLETTI (Università di Chieti-Pescara), Laura GAGLIARDI (Lincea, University of Chicago), Gianfranco PACCHIONI (Linceo, Università di Milano Bicocca), Giorgio PARISI (Linceo, Sapienza Università di Roma), Vincenzo SCHETTINO (Linceo, Università di Firenze), Roberta SESSOLI (Lincea, Università di Firenze), Antonio SGAMELLOTTI (Linceo, Università di Perugia), Adriano ZECCHINA (Linceo, Università di Torino)

Introduction

Vincenzo AQUILANTI (Linceo, Università di Perugia), Cecilia COLETTI (Università di Chieti-Pescara)

One century ago, at the birth of quantum mechanics, Dirac claimed the discovery of the founding laws of chemistry, as the science of materials at the atomic and molecular level -- however admitting that the challenge to full application needed development of efficient computational techniques. The following decade recorded the birth of information science (Von Neumann and Wigner were among founding fathers of both sciences): progress and implementations to chemistry became instrumental and today mature: Quantum Chemistry explains and predicts a variety of new phenomena, occurring in the rarefied situations of the planetary atmospheres and of the interstellar medium, and including those relevant for thermal and non-equilibrium plasmas; emerging tasks are imposed to biochemists, instrumental to life and health sciences; research is active on the electro-magnetic properties of solid conductors and semiconductors for optoelectronic applications; current Holy Grail is the chemical hardware to support exploitation of Quantum Computing. Physicochemical models at micro, meso and macro scales allow one to accumulate myriads of data that can be handled through cheminformatics approaches for the scrutiny of properties of materials or molecules, both exploiting through powerful Machine Learning methods to obtain otherwise unavailable information and to highlight through Artificial Intelligence technology correlations and universalities of behavior otherwise hidden in the non-linear equations of current complexity theory.

Thursday, 26 September

14.00 *Welcome addresses from the Presidency of the Academy*

14.15 Vincenzo AQUILANTI (Linceo, Università di Perugia), Cecilia COLETTI (Università di Chieti-Pescara): *Introduction*

Session I – Chair: Cecilia COLETTI (Università di Chieti-Pescara)

14.30 Peter M.W. GILL (University of Sidney, Australia): *Parsimonious descriptions of molecular orbitals*

15.00 Roland LINDH (Uppsala Universitet, Sweden): *Bye-bye to second-order optimization methods*

15.30 Gianfranco PACCHIONI (Linceo, Università di Milano Bicocca): *40 years in quantum chemistry: from Li clusters to nanocatalysis*

16.00 Break

16.20 Anna KRYLOV (University of Southern California, Los Angeles, USA): *In Search of Molecular Hardware for Quantum Information Science: A Quantum Chemistry Perspective*

16.50 Sonia CORIANI (Technical University of Denmark, Lyngby, Denmark): *Ab initio modeling the molecular response to light: from ultrafast (local) spectroscopy to quantum computing*

Friday, 27 September

Session II – Chair: Niyazi BULUT (Firat University, Elazig, Turkey)

9.20 Ireneusz GRABOWSKI (Nicolaus Copernicus University, Torun, Poland): *A Comprehensive Assessment of Hybrid Kohn-Sham DFT Functionals*

9.50 Valter H. CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil): *Ascent and Decline in the Temperature Dependence of Rate Processes for Biophysical Systems*

10.20 Michele CEOTTO (Università di Milano): *Unraveling Water Solvation Effects with Quantum Mechanics/Molecular Mechanics Semiclassical Vibrational Spectroscopy*

10.50 Break

Session III – Chair: Vincenzo BARONE (Scuola Normale Superiore di Pisa)

11.10 Joel M. BOWMAN (Emory University, Atlanta USA): *Permutationally Invariant Polynomial Regression is Perhaps The Fastest and Most Precise Machine Learning Method for High Dimensional Molecular Potentials*

11.40 Leonardo BELPASSI (CNR-SCITEC Perugia): *Relativistic Quantum Chemistry: past, present and future*

12.00 Loriano STORCHI (Università G. d'Annunzio, Chieti-Pescara): *Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator*

12.20 Dario DE FAZIO (CNR Montelibretti): *Artificial Quantization: Discrete Harmonics Algorithm for QRS*

12.35 Flavio Olimpio SANCHES-NETO (Instituto Federal de Educação, Ciência e Tecnologia de Goiás): *Mechanisms and Kinetics of Environmental Biocomplexity: A Quantum Chemistry and Machine Learning Perspective*

12.50 Break

14.00 Pier Luigi GENTILI (Università di Perugia): *An Unconventional Chemical Approach for the Development of Quantum Artificial Intelligence*

14.20 Alberto BAIARDI (IBM Zurich, Switzerland): *Development of Quantum Computing Algorithms for Quantum Chemistry Simulations*

14.50 Markus MEUWLY (Universitat Basel, Switzerland): *Machine Learning Models and Applications for Chemical Reactions*

15.20 Andrea LOMBARDI (Università di Perugia): *Machine learning oriented approach to few-and-many-body systems by hyperspherical coordinates and harmonics*

15.50 Hamilton BARBOSA NAPOLITANO (Universidade Estadual de Goiás): *Chalcone compounds as alternatives for fuel additives: from solid state analysis to machine learning protocols*

16.20 *Conclusions*

Parsimonious descriptions of molecular orbitals
Peter M.W. GILL (University of Sidney, Australia)

Computational chemists — scientists who predict chemical behaviour by simulating it on powerful computers — are always interested in studying larger and more complicated molecules than have been investigated previously. One of the key challenges that this poses is, "How can we describe the positions and movements of the millions of electrons in a molecule such as a large protein?" If we do not find a very compact language, such descriptions will overflow the memory of our computers. In this lecture, I will discuss an extremely parsimonious model for molecular orbitals, the functions that describe the locations of electrons in a molecule. The model is so spartan that it enables us to contemplate ten-million-electron calculations on a desktop computer with just 64 GB of memory.

Bye-bye to second-order optimization methods
Roland LINDH (Uppsala Universitet, Sweden)

The development potential of second order optimization methods has been exhausted. We need to look elsewhere as the computational chemist needs more efficient and robust optimization tool. In this presentation an alternative based on Gaussian Process Regression – a machine learning technique called Gradient Enhanced Kriging (GEK) – will be presented. We will here initially compare the characteristics of the conventional second order methods with those of GEK. The GEK will also enable a variance driven optimization approach – the Reduced Variance Optimization (RVO) strategy – an alternative to the ad hoc step-restricted optimization methods. Subsequently, we will demonstrate the superior properties of this approach for molecular structure optimizations (equilibrium and transition state structures), reaction path explorations, inter-system crossings, minimum energy Conical intersections, and SCF/DFT orbital optimizations. For the latter a subspace version of GEK (s-GEK) is proposed and implemented in which no information is lost. Finally, the s-GEK approach is shown to perform equally good regardless of the underlying 2nd order method to extend the subspace. To conclude, we think that these results demonstrate in a clear fashion that the dominance of second-order methods for optimization problem have come to an dead end. The new approach, which is still in its crib offer a new extended development potential, we invite you all to explore it together. The king is dead long live the king.

40 years in quantum chemistry: from Li clusters to nanocatalysis
Gianfranco PACCHIONI (Linceo, Università di Milano Bicocca)

I will trace the history of 40 years of research in cluster chemistry from my personal point of view recalling experiences and anecdotes in my numerous stays in Berlin, Munich, and

at IBM in California. I will describe how my research activity began in the early 1980s with studies on the electronic structure of Li clusters in the gas phase with Hartree-Fock and configuration interaction approaches. Since then, research on the chemistry and physics of clusters has made enormous progress, thanks to the development of new experimental techniques, advanced theoretical methods and a continuous growth in computing power. The structure and properties of bare clusters, ligand-stabilized organometallic clusters, and supported nanoparticles were elucidated with the ultimate goal of creating strong links between cluster science, surface chemistry, and heterogeneous catalysis. Some problems remain in the quantum chemical description of molecular and solid systems, but a much better understanding of catalysis has been gained in these years.

In Search of Molecular Hardware for Quantum Information Science: A Quantum Chemistry Perspective

Anna KRYLOV (University of Southern California, Los Angeles, USA)

To realize its technological promise, the burgeoning field of Quantum Information Science needs molecular hardware. Theoretical modeling can help in the process of search and design of suitable molecules. In this lecture I will discuss promising ideas for laser-coolable molecules, single-molecule magnets, etc. I will highlight salient aspects of the underlying electronic structure and discuss practical aspects of quantum chemistry calculations responding to the needs of QIS.

1. A.I. Krylov, The quantum chemistry of open-shell species, Reviews in Comp. Chem. 30, 151 – 224 (2017)
2. M. Alessio and A.I. Krylov, Equation-of-motion coupled-cluster protocol for calculating magnetic properties: Theory and applications to single-molecule magnets, J. Chem. Theo. Comp. 17, 4225 – 4241 (2021)
3. M.V. Ivanov, F.H. Bangerter, P. Wojcik, and A.I. Krylov, Towards ultracold organic chemistry: Prospects of laser cooling large organic molecules, J. Phys. Chem. Lett. 11, 6670 – 6676 (2020)
4. P. Wojcik, E.R. Hudson, and A.I. Krylov, On the prospects of optical cycling in diatomic cations: Effects of transition metals, spin-orbit couplings, and multiple bonds, Mol. Phys. , e2107582 (2022)

Ab initio modeling the molecular response to light: from ultrafast (local) spectroscopy to quantum computing

Sonia CORIANI (Technical University of Denmark, Lyngby, Denmark)

Spectroscopy, the most far-reaching analysis tool in chemistry, exploits the interaction of light with matter to probe molecular and electronic structures. This interaction is also the foundation of photochemistry, optogenetics, phototherapy, photocatalysis, optical devices, solar cells, and other use cases in chemistry, life sciences, and material design. The theoretical modelling and simulation of the molecular response to light thus provides crucial fundamental understanding of the microscopic mechanisms behind all spectroscopies and light-energy conversion processes.

In my talk, I will present some recent results of our research efforts concerning: (1) theoretical X-ray spectroscopy to unravel ultrafast relaxation pathways in functional molecules [1-3]; (2) the development of response algorithms for hybrid noisy intermediate-scale quantum (NISQ) computers [4-6].

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A Comprehensive Assessment of Hybrid Kohn-Sham DFT Functionals

Ireneusz GRABOWSKI (Nicolaus Copernicus University, Torun, Poland)

We present the critical evaluation of the quality of the most popular DFT hybrid functionals based on the fundamentals for Kohn-Sham DFT (KS DFT) quantities, i.e., exchange-correlation (XC) KS potentials, total energies, electron densities, and ionization potentials (IP). Our primary object in the current study is the XC potential. Since the XC potentials are not directly accessible for the hybrids, we calculate them by inverting the KS electron densities. Our study is devoted to a generalized assessment of the hybrid XC functionals available in the LIBXC library. To this end, we have tested 155 hybrid functionals. We use FCI and CCSD(T) methods as a reference in our evaluation.

Among all tested hybrid functionals, we have found that the range-separated GGA and meta-GGA ones provide the best XC potentials and IPs. [1] We also show direct and systematic dependence between the quality of IPs and the quality of XC potentials. We analyze density-driven and functional-driven errors and show that functional-driven errors dominate hybrid energy expressions. In addition, we offer that the CCSD(T) method is a sufficiently quantitative reference for this type of evaluation without the need to use expensive FCI calculations. Finally, our study [2] shows the crucial role and necessity of including XC KS potentials in developing new KS DFT functionals and evaluating existing ones.

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[2] V. Kumar, S. Śmiga, I Grabowski, submitted 2024

Ascent and Decline in the Temperature Dependence of Rate Processes for Biophysical Systems

Valter H. CARVALHO-SILVA (Universidade Estadual de Goiás, Anápolis, Brazil)

The effect of temperature on biophysical processes has been the subject of various empirical formulations, as it presents a regularity of behavior independent of the system studied: an optimal point of activity and cessation of activity for extreme temperature conditions. The description of these deviations goes beyond the conventional Arrhenius formulation, both at low temperatures where curvatures arise and at high temperatures where the apparent activation energy presents negative results. These deviations from linearity in the Arrhenius plot have been widely documented in biophysical processes with cases related to charge and mass transport properties in biochemical system – proton transfers in the catalytic reac-tion of alcohol dehydrogenase and electron flux in microbial cytochrome nanowires – and by physiological processes in living beings – heart beat and flashing of fireflies – and its implications for ecological demands – influence on soil, locomotion and growth of living organisms. In this talk, it is introduced recent studs of kinetics of a biophysical process uni-formly modeled through Generalized Transition State Theory for a series an example – a recent approach for the uniform treatment of passages between regimes of temperature de-pendence in chemistry and material science. Temperature dependence of rate coefficients is modeled, providing insight on the assembling of meso structures and unveiling the role of the prefactor in the temperature dependence of rate coefficient to account on the origin of negative activation energy. Additionally, the concept of activation heat capacity is intro-duced and generalized to account curvatures on kinetics of rate processes. The results of the cooling experiment are shown to covering smoothly the "hot" transition from the anti-regime (impulsive, stereodirected dynamics, molecular complexity) to Arrhenius thermally equilibrated regime or the "cold" deviation from Arrhenius, specifically discerning the cas-es, sub (quantum tunnel) or super (classical transport or diffusion).

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Unraveling Water Solvation Effects with Quantum Mechanics/Molecular Mechanics Semiclassical Vibrational Spectroscopy

Michele CEOTTO (Università di Milano)

Can a single classical trajectory reproduce quantum mechanical effects? Eigenfunctions, transitions between vibrational levels, zero point energy contributions, and tunneling are examples of quantum mechanical events. In this talk, I will show how the Semiclassical

Initial Value Representation (SCIVR) method is a viable tool to reproduce all of them in complex molecular systems, as molecules in condensed phase.

SCIVR is based on classical trajectory ingredients, i.e. starting from a standard molecular dynamics simulation with local Hessian calculations, and a Gaussian wavepacket is driven on the top of the classical trajectories. However, this is not enough for reproducing quantum mechanics in condensed phase. To deal with this issue and the related curse of dimensionality, I will present a Divide-and-Conquer semiclassical method that we have developed in recent years and that is allowing us to simulate complex systems with quantum mechanical accuracy using only a single classical trajectory. Specifically, I will show how the vibrational eigenfunction of the aminoacid glycine looks like or which is the smallest water drop to behave as a liquid with spectroscopic accuracy. Also, systems as complex as thymidine nucleotide solvated in a droplet of thousands of water molecules and formic acid adsorbed on a titania surface are investigated by a single classical trajectory and with nuclear quantum mechanical accuracy to unveil how important are light atom quantum delocalizations in the interplay between the solute/molecule and solvent/surface.

I will conclude that indeed one needs a quantum dynamics approach for an accurate description of molecules, even in condensed matter.

Permutationally Invariant Polynomial Regression is Perhaps The Fastest and Most Precise Machine Learning Method for High Dimensional Molecular Potentials
Joel M. BOWMAN (Emory University, Atlanta USA)

There has been a paradigm shift in using the methods of Machine Learning to represent high-dimensional molecular potentials. I will briefly outline this shift and give an overview of methods currently in use. Then I will describe a method based on Permutationally Invariant Polynomial Regression and demonstrate the speed and precision of this approach. I will give two recent applications to ethylene glycol and the hydrocarbon $C_{14}H_{30}$, where a new many-body approach will be described.

Relativistic Quantum Chemistry: past, present and future
Leonardo BELPASSI (CNR-SCITEC Perugia)

Relativistic quantum chemistry combines the principles of the special relativity with those of quantum chemistry to rationalize and predict properties, structures and reactivity of systems mainly containing heavy elements [1]. The inclusion of relativistic effects can be also important on molecules containing light atoms when the theory has to be compared with high accurate experiments. In this presentation, I will give an overview of the historical developments of the field, underlining the current trends and applications [2,3,4] and I also will give some future perspectives [5].

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Machine and Deep Learning techniques in chemistry: an overview from DeepGRID to a simple formula generator

Loriano STORCHI (Università G. d'Annunzio, Chieti-Pescara)

We will present an overview of Machine and Deep Learning techniques applied in different scenarios. Specifically, Deep Learning approaches are able to automatically extract relevant features from the input data and capture nonlinear relationships between the input and output. We present the GRID Force Field and how CNN facilitates its use to build Deep Learning models in a rotationally, conformationally, and alignment-independent approach we are calling DeepGRID [1]. Similarly we will walk though some analysis on the performance of different Machine Learning models based on the Gaussian Process or Neural Network techniques to produce complete datasets of inelastic scattering rate coefficients [2].

On the other end, we propose a combinatorial simple machine-learning approach to obtain physical formulas based on simple and easily accessible ingredients, such as atomic properties. The latter are used to build materials features that are finally employed, through linear regression, to predict the energetic stability of semiconducting binary compounds with respect to zinc blende and rocksalt crystal structures. The adopted models are trained using a dataset built from first-principles calculations [2].

Artificial Quantization: Discrete Harmonics Algorithm for QRS

Dario DE FAZIO (CNR Montelibretti)

The development of hyperspherical techniques has been crucial in the study of the dynamics of elementary chemical reactions in the gas phase. During the nineties, thanks to these advances some different algorithms capable to solve exactly the time independent Schrodinger equation for atom-diatom reactions have been developed. Their application has produced in the years a wide set of benchmark data in various energy regimes [1,2] to compare with available experimental data [3].

In the hyperquantization algorithm [4], developed in our laboratory at University of Perugia, we have used an expansion in hyperspherical harmonics to solve the eigenvalue problem at fixed radius, in a similar way as the quantum solution of the electronic levels of the hydrogen atom are solved in analytical theories. Unfortunately, the hyperspherical harmonics expansion converges slowly and a huge number of harmonics with large quantum numbers is required making the code largely inefficient. However, in the

hyperquantization algorithm this problem is by-passed by using in place of hyperspherical harmonics their discrete analogous that approximate very well the values of the hyperspherical harmonics over a grid of points when large values of the quantum numbers are involved [5]. The main advantage to use orthogonal polynomials of a discrete variable, namely the Hahn polynomials, is that exploiting the algebra of the hyperangular moments large sums among these quantities can be done analytically so that the explicit calculation of the harmonics or of the Hahn polynomials is actually not required in practice making the scattering algorithm very fast and efficient. Moreover, the mathematical properties of the Hahn polynomials permit to formulate the eigenvalue problem in terms of matrices with particular structures efficiently exploited by linear algebra methods [6].

Theoretical details of the hyperquantization algorithm and its differences with the other available methods will be presented at the conference. Results of benchmark studies carried out with this methodology in the last ten years will be also shown and discussed.

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[2] D. De Fazio, S. Cavalli and V. Aquilanti ;‘*Quantum dynamics and kinetics of the F + H_2 and F + D_2 reactions at low and ultra-low temperatures*’. *Frontiers in Chemistry,* **7** (2019) 328.

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Mechanisms and Kinetics of Environmental Biocomplexity:
A Quantum Chemistry and Machine Learning Perspective

Flavio Olimpio SANCHES-NETO (Instituto Federal de Educação,
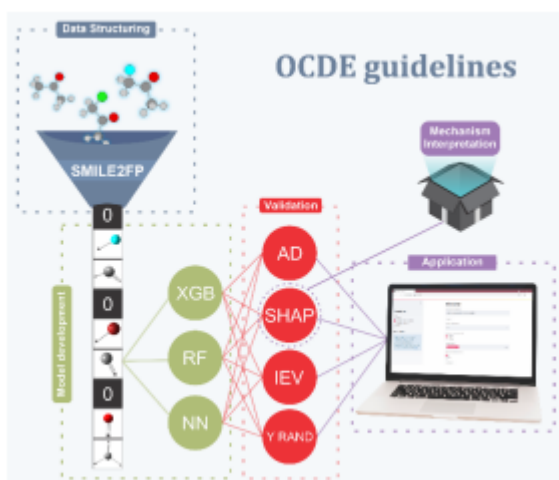Ciência e Tecnologia de Goiás)

Fig. 1. The routine follows guidelines of the Organization for Economic Cooperation and Development (OECD), see text. Data from the literature, structured and with molecular names converted by SMILES provide molecular fingerprints (MF) – these are the independent variables, while rate constants are the dependent variables of our model developed implemented in three machine learning algorithms – XGboost (XBG), Random Forest (RF), and Neural Network (NN). Validation of the model's performance involved: applicability domain (AD), mechanistic interpretation with the SHAP method, internal and external validation (IEV), and randomization of the dependent variable (Y RAND). Final step is a user-friendly web application.

Micro-pollutants of emerging concern have imposed a major technological challenge: pesticides, drugs and other anthropogenic substances are increasingly found in aquatic and atmospheric environments and even in water supplies, being related to adverse effects on biota and human health [1]. Overcoming this challenge requires understanding the behavior of these species in the environment and the development of technologies that allows for minimizing their dissemination. Viable alternatives applied in this thesis include the use of radical-based oxidation processes using both experimental – via the competition kinetics method – and theoretical protocols – blend of kinetic, quantum chemistry and machine learning calculations [2,3,4]. In a first study, the mechanisms, kinetics, and an evaluation of the toxicity of picloram degradation – a pesticide widely used in the world - initiated by OH radicals indicate that: i) two favorable pathways occur by addition to the pyridine ring, ii) picloram and the majority of degradation products are estimated as harmful; however, ii) these compounds can suffer photolysis by sunlight. However, the competition kinetic method and the quantum chemistry description make the degradation analyses a formidable enterprise, considering the costs of ad hoc instrumental equipment's and dedicated computational efforts. To overcome the demanding conventional procedures, we developed a free and user-friendly web application (www.pysirc.com.br) based on holistic machine learning combined with molecular fingerprints models that permits compilation of kinetic parameters and mechanistic interpretation of radical-based oxidation attacks according to the OECD principles. Machine learning algorithms were implemented, and all models provided high goodness-of-fit for radical-based degradation in aquatic and atmospheric environment. The models were interpreted using the SHAP (SHapley Additive exPlanations) method: the results showed that the model developed made the prediction based on a reasonable understanding of how electron-withdrawing/donating groups interfere in the reactivity of the radicals. We argue that our models and web interface can stimulate and expand the application and

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An Unconventional Chemical Approach for
the Development of Quantum Artificial Intelligence

Pier Luigi GENTILI (Università di Perugia)

Humanity is spurred to face global challenges and promote a sustainable future. Facing global challenges means dealing with Complex Systems [1]. However, we encounter many difficulties in understanding and predicting the behaviour of Complex Systems due to Epistemological Complexity [2]. A deeper comprehension and a more satisfying prediction of Complex Systems require that we face Computational Complexity and formulate universally valid and effective algorithms for recognizing variable patterns. In this regard, a promising research line is Natural Computing [2]. Within Natural Computing, two

computing strategies look particularly alluring: Quantum Computing (QC) and Artificial Intelligence (AI). Their combination has sparked the birth of Quantum Artificial Intelligence (QAI) [3].

Chemistry can contribute to Quantum Artificial Intelligence by devising innovative materials for quantum computing [4] and developing Chemical AI [5-7]. Chemical AI refers to using Molecular, Supramolecular and Systems Chemistry in liquid solutions to mimic some performances of biological intelligence. All the molecules abide by the quantum-mechanical laws. Hence, in principle, any chemical system can be exploited to encode and process qubits. However, it is well-known that decoherent phenomena hinder quantum computation, and extreme conditions are usually required to manipulate qubits. CAI proposes two alternative strategies that exploit quantum mixed states rather than qubits: one is based on the chemical implementation of fuzzy sets [8], and the other regards neuromorphic engineering in wetware [9].

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Development of Quantum Computing Algorithms
for Quantum Chemistry Simulations

Alberto BAIARDI (IBM Zurich, Switzerland)

The development of quantum-computing has currently reached the stage where hardware composed of more than 100 qubits can be constructed. Such quantum hardware – the so–called utility-scale hardware – can execute specific computational tasks that are beyond the reach of brute-force classical simulations. Designing algorithms that can maximally

harness the power of such utility-scale hardware is currently one of the primary challenges of quantum-computing research. In this contribution, I will describe novel strategies that enable exploiting utility-scale quantum computers, with a specific focus on material-science and quantum-chemical calculations.

Machine Learning Models and Applications for Chemical Reactions
Markus MEUWLY (Universitat Basel, Switzerland)

In this talk I will outline the use of machine learning techniques in Chemistry and in Physical Chemistry in particular. One more recent and rather successful application of machine learning concerns the construction of high-dimensional, reactive potential energy surfaces. The PES is arguably the most relevant object when trying to understand the underlying dynamics of chemical reactions and spectroscopy. I will discuss how such PESs can be constructed and used in classical and quantum-based simulations, with a particular emphasis on comparison with experiments.

Machine learning oriented approach to few-and-many-body systems by hyperspherical coordinates and harmonics
Andrea LOMBARDI (Università di Perugia)

In spite of the original application to few-atom systems (see e.g. [1]), hyperspherical coordinates can be derived for any number of atoms and used to represent and characterize even large molecular structures. Unlike Cartesian coordinates, the hyperspherical ones partition the degrees of freedom into shape coordinates, ordinary rotations and kinematic rotations, three groups of variables mutually invariant [2]. For this reason, they provide invariant structural information, that can be used for classification purposes in Machine Learning applications to medium and large size molecules and clusters. Here, we give a summary of the theoretical background of the coordinate and harmonics derivation for few and many-body systems and illustrate a recipe for possible use in machine learning applications.

[1] Aquilanti, V., Cavalli, S.: The quantum-mechanical hamiltonian for tetraatomic systems insymmetric hyperspherical coordinates, J. Chem. Soc. Faraday Trans. 93 (1997) 801–809.
[2] Aquilanti, V., Lombardi, A., Sevryuk, M. B.: "Phase-space invariants for aggregates of particles: Hyperangular momenta and partitions of the classical kinetic energy", J. Chem. Phys. 121, (2004) 5579–5589.

Chalcone compounds as alternatives for fuel additives: from solid state analysis to machine learning protocols

Hamilton BARBOSA NAPOLITANO (Universidade Estadual de Goiás)

Biodiesel is a promising fuel with the potential to reduce some negative aspects of fossil fuels, such as the emission of pollutants and greenhouse gases (GHG), scarcity of natural resources and market instability. To amplify its low durability and stability the use of technologies based on molecular compounds that reduce the rate of the oxidation process of biodiesel and preserve its physical-chemical properties is very common and necessary throughout the world. To reduce oxidative stability problems of diesel-biodiesel blends, chalcone compounds were evaluated as potential additives for diesel-biodiesel blends. In this study, comprehensive structural, computational, and experimental analyses were undertaken to understand the antioxidant potential of these compounds as possible additives. The supramolecular arrangements were stabilized by weak molecular interactions (C–H...O and C–H...π), that are related to antioxidant and antibacterial action, and groups can act as electron-donating substituents. The Fukui function aligned with kinetics parameters obtained by machine learning protocols propitiated information for clarifying and expanding the comprehension of chalcone antioxidant features mediated by free-radicals capture. The heat of combustion indicated good energy availability close to those of conventional fuels. Additionally, the oxidative stability in the blend (B20) remained around 27 hours, after 140 days of storage, showing better than some commercial additives. This comprehensive study supports the understanding of the chalcone-based compounds as alternatives for fuel additives

Keywords: diesel-biodiesel blends, antioxidant activity, DFT, machine learning.