

## Vincenzo Schettino - PUBBLICAZIONI

### Articoli selezionati

R Chelli, FL Gervasio, P Procacci, V Schettino

[Stacking and T-shape competition in aromatic-aromatic amino acid interactions](#)

Journal of the American Chemical Society 124 (2002), 6133-6143

[High pressure photoinduced ring opening of benzene](#)

L Ciabini, M Santoro, R Bini, V Schettino

Physical review letters 88 (2002), 085505

[Laser-induced selectivity for dimerization versus polymerization of butadiene under pressure](#)

M Citroni, M Ceppatelli, R Bini, V Schettino

Science 295 (2002), 2058-2060

[High-pressure synthesis of crystalline polyethylene using optical catalysis](#)

D Chelazzi, M Ceppatelli, M Santoro, R Bini, V Schettino

Nature materials 3 (2004), 470-475

[Metadynamics simulation of prion protein:  \$\beta\$ -structure stability and the early stages of misfolding](#)

A Barducci, R Chelli, P Procacci, V Schettino, FL Gervasio, M Parrinello

Journal of the American Chemical Society 128 (2006), 2705-2710

[Triggering dynamics of the high-pressure benzene amorphization](#)

L Ciabini, M Santoro, FA Gorelli, R Bini, V Schettino, S Rauegi

Nature Materials 6 (2007), 39-43

[Constraining molecules at the closest approach: chemistry at high pressure](#)

V Schettino, R Bini

Chemical Society Reviews 36 (2007), 869-880

[Role of excited electronic states in the high-pressure amorphization of benzene](#)

M Citroni, R Bini, P Foggi, V Schettino

Proceedings of the National Academy of Sciences 105 (2008), 7658-7663

[High-pressure photodissociation of water as a tool for hydrogen synthesis and fundamental chemistry](#)

M Ceppatelli, R Bini, V Schettino

Proceedings of the National Academy of Sciences 106 (2009), 11454-11459

[Raman and computational study of solvation and chemisorption of thiazole in silver hydrosol](#)

M Muniz-Miranda, M Pagliai, F Muniz-Miranda, V Schettino

Chemical Communications 47 (2011), 3138-3140

### Articoli scientifici

1. Antonio Sabatini, Luigi Sacconi, Vincenzo Schettino  
*Far-infrared spectra and vibrational force constants of the ions  $PtCl_4^-$ ,  $AuCl_4^-$  and  $AuBr_4^-$ -Inorg. Chem. **3** (1964) 1775*
2. Vincenzo Schettino, Natale Neto, Salvatore Califano  
*Crystal spectra in polarized light, vibrational assignment and force constants calculation of phenanthrene.*  
J Chem. Phys. **44** (1966) 2724

3. Mario P. Marzocchi, Vincenzo Schettino, Salvatore Califano  
*Infrared spectrum of crystalline CH<sub>2</sub>I<sub>2</sub>. Crystal spectrum and phase transition.*  
J. Chem. Phys. **45** (1966) 1400
4. J.H. Fertel, C.H. Perry, A. Sabatini, L. Sacconi, V. Schettino  
*Correction to paper "Long-wave infrared spectra of alkali salts of Platinum Halide Complexes"*  
J. Chem. Phys. Solids, 27 (1966) 1551
5. Vincenzo Schettino  
*Vibrational assignment of phenanthrene-d<sub>10</sub>*  
J. Chem. Phys. **46** (1967) 302
6. Enzo Benedetti, Sergio Pucci, Piero Pino, Vincenzo Schettino, Salvatore Califano  
*Vibrational spectra of model compounds of polypropylene. I. Infrared spectra and rotational isomerism in H(CH<sub>2</sub>CHMe) nMe, (n=2, 3, 4)*  
Spectrochim. ActaA **23(8)** (1967) 2371-81
7. Vincenzo Schettino, M. P. Marzocchi, Giuseppe Sbrana  
*Vibrational crystal spectrum of [2.2]paracyclophane*  
J. Mol. Struct. **2(1)** (1968) 39-45
8. M. P. Marzocchi, Paolo Manzelli, Vincenzo Schettino, Salvatore Califano  
*Infrared spectrum in polarized light of dibromomethane and dideuteriodibromomethane. Determination of the crystal structure*  
J. Chem. Phys. **49(12)** (1968) 5438-44
9. Vincenzo Schettino  
*Molecular interactions in crystals*  
Corsi Semin. Chim. **No. 14** (1968) 62
10. Isamu C. Hisatsune, Riccardo Passerini, R. Pichai, Vincenzo Schettino  
*Thermal isomerization of the maleate ion in potassium halide matrixes*  
J. Phys. Chem. **73(11)** (1969) 3680-2
11. Vincenzo Schettino, M. P. Marzocchi, Salvatore Califano  
*Infrared spectra of crystalline cyclopentane and cyclopentane-d<sub>10</sub>*  
J. Chem. Phys. **51(12)** (1969) 5264-76
12. Sbrana, Giuseppe, Vincenzo Schettino  
*Vibrational spectra and isomerism in propion- and butyraldehyde*  
J. Mol. Spectrosc. **33(1)** (1970) 100-8
13. Vincenzo Schettino, I. C. Hisatsune  
*Infrared spectrum of matrix-isolated cyanate ion. I. Vibrational analysis, bandwidths, and absolute intensities in potassium halides*  
J. Chem. Phys. **52(1)** (1970) 9-27
14. Vincenzo Schettino  
*Infrared and Raman spectra of crystalline triphenylene and triphenylene-d<sub>12</sub> and normal coordinates calculations*  
J. Mol. Spectrosc. **34(1)** (1970) 78-96
15. Giuseppe Sbrana, Pier F. Franchini, Vincenzo Schettino  
*Molecular structure of 5, 5'-biisoxazole. 1. Vibrational assignment and dipole measurement*  
Trans. Faraday Soc. **66(3)** (1970) 563-71
16. Vincenzo Schettino, Giuseppe Sbrana, Roberto Righini  
*Evidence for a phase transition in crystalline pyrazine*  
Chem. Phys. Lett. **13(3)** (1972) 284-5
17. Vincenzo Schettino, M. P. Marzocchi  
*Laser Raman spectrum of crystalline cyclopentane-d<sub>0</sub> and -d<sub>10</sub>*  
J. Chem. Phys. **57(10)** (1972) 4225-9
18. Vincenzo Schettino  
*One- and two-phonon spectra of crystalline silicon tetrafluoride*  
Chem. Phys. Lett. **18(4)** (1973) 535-9

19. Dows, David A., Vincenzo Schettino  
*Two-phonon infrared absorption spectra in crystalline carbon dioxide*  
J. Chem. Phys. **58(11)** (1973) 5009-16
20. Benedetti, E., Pucci, S., Pino, P., Vincenzo Schettino  
*Vibrational spectra of model compounds of polypropylene. II. Infrared spectra and rotational isomerism of 2, 4, 6, 8, 10- pentamethylundecane*  
Spectrochim. ActaA **29(7)** (1973) 1313-20
21. Giuseppe Sbrana, Vincenzo Schettino, Roberto Righini  
*Phase transition in crystalline pyrazine. Infrared and Raman spectra*  
J. Chem. Phys. **59(5)** (1973) 2441-50
22. D. P. Craig, Vincenzo Schettino  
*2X . nu. 3 transition in crystal tetrafluorosilane*  
Chem. Phys. Lett. **23(3)** (1973) 315-17
23. David A. Dows, Vincenzo Schettino  
*Two-phonon absorption in the  $\nu_1 + \nu_2$ ,  $2\nu_2 + \nu_2$  region of carbon dioxide crystal*  
Spectrochim. ActaA **30A(7)** (1974) 1451-3
24. Vincenzo Schettino, Robert E. Salomon  
*Infrared and Raman spectra of crystalline hydrazinium monochloride*  
Spectrochim. ActaA **30 (7)** (1974) 1445-50
25. Vincenzo Schettino  
*Two-phonon absorption in silicon tetrafluoride*  
in *Lattice Dynamics and Intermolecular Forces*, Academic Press **55** (1975) 326-41
26. Vincenzo Schettino, Pier Remigio Salvi  
*Cooperative excitations and infrared absorption in nitrous oxide crystals*  
Spectrochim. Acta **31A** (1975) 399-410
27. Vincenzo Schettino, Pier Remigio Salvi  
*Phonon energies and absorption processes in carbonyl sulphide crystals*  
Spectrochim. Acta **31A** (1975) 411-420
28. Cangeloni, M. L., Vincenzo Schettino  
*Infrared and Raman spectra and polymorphism in crystal n-butane*  
Mol. Cryst. Liq. Cryst. **31(3-4)** (1975) 219-31
29. Pier Remigio Salvi, Roberto Righini, Vincenzo Schettino  
*Phonon side bands of molecular crystal excitons*  
in *Molecular Spectroscopy of dense phases*, Elsevier (1976) 177-180
30. Roberto Righini, Pier Remigio Salvi, Vincenzo Schettino  
*Coupled phonon modes and infrared band shapes in crystal SiF<sub>4</sub>*  
Molec. Cryst. Liq. Cryst. **43** (1977) 223-234
31. Pier Remigio Salvi, Roberto Righini, Vincenzo Schettino  
*Lattice dynamics and phonon sidebands of vibrational excitons in carbonyl sulphide crystal*  
J. Phys. C **10** (1977) 11-21
32. Emilio Castellucci, Vincenzo Schettino  
*Raman spectrum of ferroelectric sodium nitrite. Angular dispersion and lattice dynamics calculations.*  
VI International Conference on Raman Spectroscopy (1978)
33. Bogani, F., Vincenzo Schettino  
*Dipole-dipole interaction and internal vibrations in molecular crystals*  
J. Phys. C **11(7)** (1978) 1275-81
34. Vincenzo Schettino, Benedetti, E.  
*Infrared and Raman spectra and normal frequencies calculation of isomeric (+) (S) -1-chloro-2-methylbutane*  
Spectrochim. ActaA **34A(3)** (1978) 353-6

35. Guasti, R., Vincenzo Schettino, Brigot, N.  
*The structure of carbon dioxide dimers trapped in solid rare gas matrices*  
Chem. Phys. **34(3)** (1978) 391-8
36. Raffaele G. Della Valle, P. Francesco Fracassi, Vincenzo Schettino, Salvatore Califano  
*Anharmonic interactions in molecular crystals. Two-phonon absorption in crystalline OCS*  
Chem. Phys. **43** (1979) 385
37. E. Castellucci, Vincenzo Schettino  
*Angular dispersion of the internal phonon modes in ferroelectric sodium nitrite*  
Phys. Status Solidi B **91(2)** (1979) 641-5
38. Pier Remigio Salvi, Vincenzo Schettino  
*Infrared and Raman spectra and phase transition of the SF<sub>6</sub> crystal. Anharmonic interactions and two-phonon infrared absorption*  
Chem. Phys. **40** (1979) 413-424
39. Vincenzo Schettino, Pier Remigio Salvi  
*The internal vibration of the hydrogen chloride crystal: electrostatic interactions and infrared bandshape*  
Chem. Phys. **41** (1979) 439-447
40. Vincenzo Schettino, Salvatore Califano  
*Theory of infrared and Raman intensity of the lattice vibrations of molecular crystals. Application to solid ammonia and benzene*  
J. Chim. Phys. Phys. -Chim. Biol. **76(2)** (1979) 197-204
41. Vincenzo Schettino  
*The effect of multiphonon processes on vibrational band shapes in molecular solids*  
NATO Adv. Study Inst. Ser. B **56** (1980) 405-14
42. E. Castellucci, Vincenzo Schettino  
*Lattice dynamics of ferroelectric sodium nitrite*  
J. Mol. Struct. **61** (1980) 191-4
43. Marco Maestro, Vincenzo Schettino  
*The infrared spectra of the cyclic depsipeptides (LMeVal-DHylv) 2 and (LMeVal-LHylv) 2*  
J. Chim. Phys. Phys. -Chim. Biol. **78(6)** (1981) 567-9
44. Salvatore Califano, Vincenzo Schettino  
*The intensity of infrared and Raman bands in molecular crystals*  
Stud. Phys. Theor. Chem. **20** (1982) 417-48
45. Vincenzo Schettino, Salvatore Califano  
*Infrared and Raman spectra of molecular crystals*  
Adv. Infrared Raman Spectrosc. **10** (1983) 219-76
46. Vincenzo Schettino, Salvatore Califano  
*Lattice dynamics and interaction potentials in molecular crystals*  
J. Mol. Struct. **100** (1983) 459-83
47. Gianni Cardini, Vincenzo Schettino  
*The HCl stretching vibration in HCl/DCI Mixed Crystal*  
Mol. Cryst. Liq. Cryst. Letters **92** (1983) 15-22
48. Giua, Roberto, Vincenzo Schettino  
*Polarization interactions in lattice dynamics of molecular crystals*  
Chem. Phys. Lett. **105(1)** (1984) 86-90
49. Franco Bogani, Roberto Giua, Vincenzo Schettino  
*Two-exciton spectra of hydrogen chloride and hydrogen bromide crystals*  
Chem. Phys. **88(3)** (1984) 375-89
50. Gianni Cardini, Vincenzo Schettino  
*Raman Intensity of Lattice Vibration in Naphtalene*  
J. Raman Spectroscopy **15** (1984) 237-240
51. Roberto Righini, Vincenzo Schettino  
*Second order Raman scattering in molecular crystals. Phonon side bands in crystalline*

*carbon disulfide*

- J. Chim. Phys. Phys. -Chim. Biol. **82(2-3)** (1985) 183-90
52. Franco Bogani, Gianni Cardini, Vincenzo Schettino, Pier Lorenzo Tasselli  
*Vibrational relaxation of two phonon bound states in molecular crystals*  
in *Dynamics of Molecular Crystals*, Elsevier (1987) 99-104
53. Gianni Cardini, Pier Remigio Salvi, Vincenzo Schettino  
*Anharmonic Interactions and Fermi Resonance in Crystal CS<sub>2</sub>*  
Chem. Phys. **117** (1987) 341-353 [[cs2.tex](#) / [other files](#)]
54. Franco Bogani, Gianni Cardini, Vincenzo Schettino and Pier Luigi Tasselli  
*Vibrational relaxation of Fermi doublets in the Raman spectra of molecular crystals*  
in *XI International Conference on Raman Spectroscopy*, Wiley (1978)
55. Salvatore Califano, Vincenzo Schettino  
*Vibrational relaxation in molecular crystals*  
Int. Rev. Phys. Chem. **7(1)** (1988) 19-57
56. Gianni Cardini, Pier Remigio Salvi, Vincenzo Schettino  
*Biphonons in crystal N<sub>2</sub>O*  
Chem. Phys. **119** (1988) 241-251
57. Vincenzo Schettino  
*Vibrations of crystal lattices*  
NATO ASI Ser. C **288** (1989) 21-51
58. Gianni Cardini, Vincenzo Schettino, Michael L. Klein  
*Structure and Dynamics of carbon dioxide clusters: a Molecular Dynamics study*  
J. Chem. Phys. **90** (1989) 4441-4449
59. Gianni Cardini, Pier Remigio Salvi, Vincenzo Schettino, Hans J. Jodl  
*Pressure tuning of Fermi resonance in crystal CO<sub>2</sub>: the solid state approach*  
J. Chem. Phys. **91** (1989) 3869-3876
60. Leonardo Angeloni, Roberto Righini, Pier Remigio Salvi, Vincenzo Schettino  
*Relaxation dynamics of Fermi doublets in CS<sub>2</sub> crystal*  
Chem. Phys. Letters **154** (1989) 432-438
61. Roberto Bini, Paolo Foggi, Pier Remigio Salvi, Vincenzo Schettino, Hans J. Jodl  
*High resolution FT-IR studies of vibrational relaxation in molecular crystals*  
in *International Workshop on Fourier Transform Infrared Spectroscopy*, Antwerp (1990)
62. Gianni Cardini, Vincenzo Schettino  
*Molecular Dynamics simulation of the vibrational properties of disordered N<sub>2</sub>O crystal: I Lattice frequencies*  
J. Chem. Phys. **93** (1990) 1973-1980
63. Franco Bogani, Gianni Cardini, Vincenzo Schettino, Pier Lorenzo Tasselli  
*Vibrational relaxation and dephasing of two-phonon bound states in molecular crystals*  
Phys. Rev. **B42** (1990) 2307-2324 [[bound.pdf.gz](#)]
64. Gianni Cardini, Vincenzo Schettino  
*Normal modes analysis in molecular dynamics simulations: Application to model alkanes*  
Chem. Phys. **146** (1990) 147-153
65. Roberto Bini, Paolo Foggi, Pier Remigio Salvi, Roberto Simone, Vincenzo Schettino  
*Vibrational relaxation of Davydov components of the 940 cm<sup>-1</sup> mode in KClO<sub>4</sub> crystal*  
J. Mol. Struct. **219** (1990) 43-48
66. Roberto Bini, Paolo Foggi, Pier Remigio Salvi, Vincenzo Schettino  
*FTIR study of vibrational relaxation in KClO<sub>4</sub> crystal*  
J. Phys. Chem. **94** (1990) 6653-6658
67. Gianni Cardini, Vincenzo Schettino  
*Molecular Dynamics simulation of the vibrational properties of disordered N<sub>2</sub>O crystal: II nu<sub>1</sub> mode.*  
J. Chem. Phys. **94** (1991) 2502-2508

68. Franco Bogani, Gianni Cardini, Vincenzo Schettino  
*Vibrational relaxation and dephasing of Fermi resonance states in molecular crystals*  
J. Chem. Phys. **95** (1991) 2523-2536
69. Roberto Bini, Pier Remigio Salvi, Vincenzo Schettino, Hans J. Jodl  
*Triphonons in crystal CO<sub>2</sub>*  
Phys. Letters A **157** (1991) 273-282
70. Giorgio F. Signorini, Roberto Righini, Vincenzo Schettino  
*Lattice dynamics of the orthorhombic phase of KClO<sub>4</sub>: Ewald's method in molecular coordinates*  
Chem. Phys. **154** (1991) 245-261
71. Paolo Foggi, Vincenzo Schettino  
*Vibrational relaxation in crystals: theory and experiments*  
Rivista Nuovo Cimento **15** (1992) 1-82
72. C. Taiti, Paolo Foggi, Renato Torre, Vincenzo Schettino  
*The CARS excitation profile of the MnO<sub>4</sub><sup>-</sup> ion doped in KClO<sub>4</sub>*  
Chem. Phys. Lett. **199** (1992) 417-422
73. Piero Procacci, Gianni Cardini, Pier Remigio Salvi, Vincenzo Schettino  
*Vibrational frequencies of C<sub>70</sub>*  
Chem. Phys. Letters **195** (1992) 347-351
74. Gianni Cardini, Piero Procacci, Pier Remigio Salvi, Vincenzo Schettino  
*Vibrational properties of Xe-fullerenes adducts: a Molecular Dynamics approach*  
Chem. Phys. Letters **200** (1992) 39-45
75. Gianni Cardini, Vincenzo Schettino  
*A molecular-dynamics study of the isotopic substitution effects on the lineshape of an internal mode in a molecular crystal*  
Chem. Phys. Letters **200** (1992) 552-558
76. Roberto Bini, Pier Remigio Salvi, Vincenzo Schettino, Hans J. Jodl, Nada Orlic  
*Vibrational relaxation of three-phonon bound states in crystal CO<sub>2</sub>*  
J. Mol. Struct. **266** (1992) 165-170
77. Gianni Cardini, Piero Procacci, Pier Remigio Salvi, Vincenzo Schettino  
*Molecular dynamics simulation of rare gas fullerene adducts.*  
Low Temperature Physics **19** (1993) 562-566
78. Roberto Bini, Pier Remigio Salvi, Vincenzo Schettino, Hans J. Jodl  
*The spectroscopy and relaxation dynamics of three-phonon bound states in crystal CO<sub>2</sub>*  
J. Chem. Phys. **98** (1993) 164-177
79. Roberto Bini, Piero Procacci, Pier Remigio Salvi, Vincenzo Schettino  
*The Far infrared spectrum of C<sub>60</sub>*  
J. Phys. Chem. **97** (1993) 10580-10584
80. Claudia Taiti, Paolo Foggi, Giorgio F. Signorini, Vincenzo Schettino  
*Vibrational relaxation of a MnO<sub>4</sub><sup>-</sup> impurity mode in KClO<sub>4</sub> crystal*  
Chem. Phys. Lett. **212** (1993) 283-288
81. Claudia Taiti, Paolo Foggi, Renato Torre, Vincenzo Schettino  
*The CARS excitation profile of the MnO<sub>4</sub><sup>-</sup> ion doped in KClO<sub>4</sub>*  
in *Coherent Raman Spectroscopy*, World Scientific (1993)
82. Claudia Taiti, Paolo Foggi, Giorgio F. Signorini, Vincenzo Schettino  
*Linewidth temperature dependence of the nu<sub>1</sub> mode of MnO<sub>4</sub><sup>-</sup> ion doped in KClO<sub>4</sub> crystal*  
in *Coherent Raman Spectroscopy*, World Scientific (1993)
83. Gianni Cardini, R. Bini, P. R. Salvi, Vincenzo Schettino, M. L. Klein, Robert M. Strongin, Laurent Brard, Amos B. Smith III  
*The infrared spectrum of two fullerene derivatives: C<sub>60</sub>O and C<sub>60</sub>H<sub>2</sub>*  
J. Phys. Chem. **98** (1994) 9966-9971

84. Vincenzo Schettino, Pier Remigio Salvi, Roberto Bini, Gianni Cardini  
*On the vibrational assignment of fullerene C<sub>60</sub>*  
J. Chem. Phys. **101** (1994) 11079-11081
85. Cristina Panero, Roberto Bini, Vincenzo Schettino  
*Vibron dynamics in Naphthalene crystal*  
J. Chem. Phys. **100** (1994) 7938-7944
86. Leonardo Poletti, Roberto Bini, Vincenzo Schettino  
*Vibrational relaxation of lattice phonons in CS<sub>2</sub> crystal*  
Chem. Phys. Lett. **222** (1994) 239-244
87. Roberto Bini, Sergio Corti, Paolo Foggi, Vincenzo Schettino, G. Buntix, O. Poizat  
*The study of conformations of 1-phenyl- and 2-phenyl-naphthalene in the triplet state by transient absorption and Raman spectroscopies*  
VII International Conference on Time Resolved Vibrational Spectroscopy (1995)
88. Barbara Caldarone, Claudia Taiti, Roberto Bini, Vincenzo Schettino  
*Vibrational relaxation in disordered 1, 4-dihalobenzenes*  
J. Chem. Phys. **102** (1995) 6653-6659
89. Cristina Gellini, Pier Remigio Salvi, Vincenzo Schettino  
*Vibrational relaxation of multiphonon bound states in disordered crystals*  
in *Fast elementary processes in chemical and biological systems*, American Institute of Physics **364** (1996) 181-190
90. Alessandro Vigiani, Gianni Cardini, Vincenzo Schettino  
*A molecular dynamics study of the CO<sub>2</sub> / NaCl (001) system.*  
J. Chem. Phys. **106** (1997) 5693-5705
91. Simone Raugai, Gianni Cardini, Vincenzo Schettino, Hans J. Jodl  
*Orientalional ordering in the mixed crystal Ar<sub>1-x</sub>(N<sub>2</sub>)<sub>x</sub>: a molecular dynamics study*  
J. Chem. Phys. **106** (1997) 8196-8203
92. Cristina Gellini, Pier Remigio Salvi, Vincenzo Schettino  
*Vibrational relaxation of multiphonon bound states in crystalline HCl*  
J. Chem. Phys. **106** (1997) 6942-6946
93. Cristina Gellini, Pier Remigio Salvi, Vincenzo Schettino, Hans-Jorg Jodl  
*Three-phonon vibrational complexes in crystal N<sub>2</sub>O*  
Chem. Phys. Letters **268** (1997) 381-38695
94. Francesco Luigi Gervasio, Gianni Cardini, Pier Remigio Salvi and Vincenzo Schettino  
*The low-frequency vibrations of all-trans-retinal: far-infrared and Raman spectra and density functional calculations*  
J. Phys. Chem. A **102** (1998) 2131-2136
95. Simone Raugai, Gianni Cardini, Vincenzo Schettino, Hans J. Jodl  
*A molecular dynamics simulation of the vibrational properties of the Ar<sub>1-x</sub>(N<sub>2</sub>)<sub>x</sub> crystal*  
J. Chem. Phys. **109** (1998) 6382-6389
96. Simone Raugai, Gianni Cardini, Vincenzo Schettino  
*Intermolecular interactions in the N<sub>2</sub>-N<sub>2</sub> dimer.*  
Mol. Phys. **95** (1998) 477-482
97. Vincenzo Schettino, Francesco Luigi Gervasio and Gianni Cardini, Pier Remigio Salvi  
*Density functional calculation of structure and vibrational spectra of polyenes*  
J. Chem. Phys. **110** (1999) 3241-3250
98. Simone Raugai, Gianni Cardini and Vincenzo Schettino  
*An ab-initio molecular dynamics study of the S<sub>N</sub>2 reaction Cl<sup>-</sup> + CH<sub>3</sub>Br -> CH<sub>3</sub>Cl + Br<sup>-</sup>*  
J. Chem. Phys. **111** (1999) 10887-10894
99. Francesco Luigi Gervasio, Piero Procacci, Gianni Cardini, Antonio Guarna, Alessandro Giolitti and Vincenzo Schettino  
*The interaction between aromatic residues: molecular dynamics and ab initio exploration of the potential energy surface of the tryptophan-histidine pair*  
J. Phys. Chem. A **104** (2000) 1108-1114

- 100 Riccardo Chelli, Francesco L. Gervasio, C. Gellini, P. Procacci, G. Cardini, and V. Schettino  
*Density functional calculation of structural and vibrational properties of glycerol*  
J. Phys. Chem. A **104** (2000) 5351-5357
- 101 Riccardo Chelli, Francesco L. Gervasio, Cristina Gellini, Piero Procacci, Gianni Cardini, Vincenzo Schettino  
*Conformational distribution of gas-phase glycerol*  
J. Phys. Chem. A **104** (2000) 11220-11222
- 102 Laura Moroni, Cristina Gellini, Pier Remigio Salvi, Vincenzo Schettino  
*Fluorescence of all-trans-Retinal as a Crystal and in a Dense Solution Phase*  
J. Phys. Chem. A **104** (2000) 11063-11069
- 103 M. Ceppatelli, M. Santoro, Roberto Bini, V. Schettino  
*FTIR study of the pressure and laser induced polymerization of solid acetylene.*  
J. Chem. Phys. **113** (2000) 5991
- 104 F. L. Gervasio, R. Chelli, M. Marchi, P. Procacci, V. Schettino  
*Determination of the potential of mean force of aromatic amino acid complexes in various solvents using molecular dynamics simulations: The case of the tryptophan-histidine pair*  
J. Phys. Chem. B **105** (2001) 7835-7846
- 105 Simone Raugei, Gianni Cardini and Vincenzo Schettino  
*Microsolvation effect on chemical reactivity: the case of  $Cl^- + CH_3Br$   $S_N2$  reaction*  
J. Chem. Phys. **114** (2001) 4089-4098
- 106 Marco Pagliai, Simone Raugei, Gianni Cardini and Vincenzo Schettino  
*Ab-initio Molecular Dynamics of the  $S_N2$  reaction:  $Cl^- + ClCH_2CN$*   
Phys. Chem. Chem. Phys. **3** (2001) 2559-2566
- 107 Marco Capecchi, Roberto Bini, Gianni Cardini, Vincenzo Schettino  
*The vibrational spectra of phosphorous oxynitride at high pressure in Oxide-Based Systems at the Crossroad of Chemistry*, ed. A. Gamba and C. Coletta and S. Coluccia, Elsevier Science B. V. (2001)
- 108 Lucia Ciabini, L. Santoro, Roberto Bini, Vincenzo Schettino  
*High pressure crystal phases of benzene probed by infrared spectroscopy*  
J. Chem. Phys. **115** (2001) 3742-3749
- 109 Marco Pagliai, Simone Raugei, Gianni Cardini, Vincenzo Schettino  
*Car-Parrinello molecular dynamics of the  $S_N2$  reaction  $Cl^- + Cl_2CH_2$*   
Phys. Chem. Chem. Phys. **3** (2001) 4870-4873
- 110 Vincenzo Schettino, Marco Pagliai, Lucia Ciabini, Gianni Cardini  
*The Vibrational Spectrum of fullerene  $C_{60}$*   
J. Phys. Chem. A **105** (2001) 11192-11196
- 111 Francesco Luigi Gervasio, Vincenzo Schettino, Paolo Carloni, Michele Parrinello  
*Fine Tuning of Zn-enzyme Chemistry: The Case of Horse Liver Alcohol Dehydrogenase*  
J. Inorg. Biochem. (2001) 233
- 112 L. Moroni, C. Gellini, P.R. Salvi, and V. Schettino  
*Ab initio structural calculations of medium-sized molecular systems*  
in Science and Supercomputing at CINECA, 2001 Report, Eds M. Voli, M. Moretti, F. Garofalo, Bologna 2001
- 113 R. Chelli, F. L. Gervasio, P. Procacci, V. Schettino  
*Stacking and T-shape competition in aromatic-aromatic amino acid interactions*  
J. Am. Chem. Soc. **124** (2002) 6133-6143
- 114 Francesco L. Gervasio, Riccardo Chelli, Piero Procacci, Vincenzo Schettino  
*Is the T-shaped toluene dimer a stable intermolecular complex?*  
J. Phys. Chem. A **106** (2002) 2945-2948
- 115 Vincenzo Schettino, Marco Pagliai, Gianni Cardini  
*The Infrared and Raman Spectra of Fullerene  $C_{70}$ . DFT calculations and correlation with  $C_{60}$ .*  
J. Phys. Chem. A **106** (2002) 1815-1823



- 116 Lucia Ciabini, M. Santoro, Roberto Bini, Vincenzo Schettino  
*High pressure reactivity of solid benzene probed by infrared spectroscopy*  
J. Chem. Phys. **116** (2002) 2928-2935
- 117 Lucia Ciabini, M. Santoro, Roberto Bini, Vincenzo Schettino  
*High pressure photoinduced ring opening and amorphization of solid benzene*  
Phys. Rev. Letters **88** (2002) 085505
- 118 Marco Pagliai, Simone Raugai, Gianni Cardini, Vincenzo Schettino  
*Thermal effects on the  $Cl^- + ClCH_2CN$  reaction by Car-Parrinello Molecular Dynamics*  
J. Chem. Phys. **117** (2002) 2199-2204
- 119 M. Citroni, M. Ceppatelli, Roberto Bini, V. Schettino  
*Laser-Induced Selectivity for Dimerization versus Polymerization of Butadiene under Pressure*  
Science **295** (2002) 2058-2060
- 120 M. Citroni, M. Ceppatelli, Roberto Bini, Vincenzo Schettino  
*IR Study of the pressure induced solid state di- and polymerization in 1, 3-Butadiene*  
High Press. Res. **22** (2002) 507-510
- 121 Francesco L. Gervasio, Riccardo Chelli, Piero Procacci, Vincenzo Schettino  
*The nature of intermolecular interactions between aromatic amino acid residues*  
Proteins **48** (2002) 117-125
- 122 Martina Mugnai, Gianni Cardini, Vincenzo Schettino  
*An ab-initio molecular dynamics study of the  $S_N2$  reaction  $F^- + CH_3Cl \rightarrow CH_3F + Cl^-$*   
J. Chem. Phys. **118** (2003) 2767-2774
- 123 Marco Pagliai, Simone Raugai, Gianni Cardini, Vincenzo Schettino  
*Car-Parrinello Molecular Dynamics on the  $S_N2$  reaction  $Cl^- + CH_3Br$  in water*  
J. Mol. Struct: THEOCHEM **630** (2003) 141-149
- 124 M. Ceppatelli, M. Santoro, Roberto Bini, Vincenzo Schettino  
*High pressure reactivity of solid furan probed by infrared and Raman spectroscopy*  
J. Chem. Phys. **118** (2003) 1499-1506
125. Citroni, M. Ceppatelli, Roberto Bini, Vincenzo Schettino  
*Phase-diagram and crystal phases of trans-1, 3 butadiene probed by FTIR and Raman spectroscopy.*  
Chem. Phys. Letters. **367** (2003) 186-192
- 126 M. Citroni, M. Ceppatelli, Roberto Bini, Vincenzo Schettino  
*The high-pressure chemistry of butadiene crystal.*  
J. Chem. Phys. **118** (2003) 1815-1820
- 127 Martina Mugnai, Gianni Cardini, Vincenzo Schettino  
*The Substitution and Elimination Reaction of  $F^-$  with  $C_2H_5Cl$ : An Ab-Initio Molecular Dynamics Study*  
J. Phys. Chem. A **107** (2003) 2540-2547
- 128 Marco Pagliai, Gianni Cardini, Roberto Righini, Vincenzo Schettino  
*Hydrogen bond dynamics in liquid methanol*  
J. Chem. Phys. **119** (2003) 6655-6662
- 129 Marco Pagliai, Simone Raugai, Gianni Cardini, V. Schettino  
*Intramolecular solvation effects in the  $S_N2$  reaction  $Cl^- + Cl(CH_2)_nCN$*   
J. Chem. Phys. **119** (2003) 9063-9072
- 130 M. Santoro, M. Ceppatelli, Roberto Bini, Vincenzo Schettino  
*High pressure photo-chemistry of furan crystal*  
J. Chem. Phys. **118** (2003) 8321-8325
- 131 M. Santoro, L. Ciabini, Roberto Bini, Vincenzo Schettino  
*High pressure polymerisation of phenylacetylene and of the benzene and acetylene moieties*  
J. Raman Spectrosc. **34** (2003) 557-566
- 132 Vincenzo Schettino, Roberto Bini  
*Matter under extreme conditions: chemical reactions at high pressure*  
Phys. Chem. Chem. Phys. **5** (2003) 1951-1965

- 133 F. L. Gervasio, Vincenzo Schettino, S. Mangani, M. Krack, P. Carloni, M. Parrinello  
*Influence of outer-shell metal ligands on the structural and electronic properties of horse liver alcohol dehydrogenase zinc active site*  
J. Phys. Chem. B **107** (2003) 6886-6892
- 134 Maurizio Muniz-Miranda, Gianni Cardini, Vincenzo Schettino  
*Surface-enhanced Raman spectra of pyridine and pyrazolide on silver colloids: chemical and electromagnetic effects*  
Theo. Chem. Acc. **111** (2004) 264-269
- 135 Martina Mugnai, Gianni Cardini, Vincenzo Schettino  
*High pressure reactivity of propene by first principles molecular dynamics calculations*  
J. Chem. Phys. **120** (2004) 5327-5333
- 136 . Martina Mugnai, Gianni Cardini, Vincenzo Schettino  
*Charge separation and polymerization of hydrocarbons at ultrahigh pressure*  
Phys. Rev. B **70** (2004) 020101(1) -020101(4)
- 137 Giorgio F. Signorini, Riccardo Chelli, Piero Procacci, Vincenzo Schettino  
*Energetic fitness of histidine protonation states in PDB structures*  
J. Phys. Chem. B **108** (2004) 12252-12257
- 138 . R.Chelli, F. L. Gervasio, P. Procacci, V. Schettino  
*Inter-residue and solvent-residue interactions in proteins: a statistical study on experimental structures*  
PROTEINS **55** (2004) 139-151
- 139 Martina Mugnai, Gianni Cardini, Vincenzo Schettino  
*Ab-initio molecular dynamics study of the potential energy surface for the  $CH_3Cl + F^-$  reaction*  
Rend. Fis. Acc. Lincei **s. 9, 15** (2004) 99-113
- 140 David Chelazzi, M. Ceppatelli, M. Santoro, Roberto Bini, Vincenzo Schettino  
*High pressure synthesis of crystalline polyethylene by using an optical catalysis*  
Nature materials **3** (2004) 470-475
- 141 Maurizio Muniz-Miranda, Gianni Cardini, Vincenzo Schettino  
*SERS and DFT study on 4-methylpyridine adsorbed on silver colloid and electrode*  
J. Phys. Chem. B **108** (2004) 17007-17011
- 142 Riccardo Chelli, Marco Pagliai, Piero Procacci, Gianni Cardini, Vincenzo Schettino  
*Polarization response of water and methanol investigated by a polarizable force field and density functional theory calculations: implications for charge transfer*  
J. Chem. Phys. **122** (2005) 074504
- 143 Marco Pagliai, Gianni Cardini, Vincenzo Schettino  
*The solvation dynamics of  $Li^+$  and  $Cl^-$  ions in liquid methanol*  
J. Phys. Chem. B **109** (2005) 7475-7481
- 144 A. Barducci, R. Chelli, P. Procacci, V. Schettino  
*Misfolding pathways of the prion protein probed by molecular dynamics simulations*  
Biophys. J. **88** (2005) 1334-1343
- 145 David Chelazzi, M. Ceppatelli, M. Santoro, Roberto Bini, Vincenzo Schettino  
*Pressure-induced polymerization in solid ethylene*  
J. PHYS. CHEM. B **109** (2004) 21658-21663
- 146 R. Chelli, A. Barducci, Luca Bellucci, V. Schettino, P. Procacci  
*Behavior of polarizable models in presence of strong electric fields. I. Origin of nonlinear effects in water point-charge systems*  
J. Chem. Phys. **123** (2005) 194109
- 147 R. Chelli, V. Schettino, P. Procacci  
*Comparing polarizable force fields to ab initio calculations reveals nonclassical effects in condensed phases*  
J. Chem. Phys. **122** (2005) 234107
- 148 V. Schettino, R. Bini, M. Ceppatelli, L. Ciabini, M. Citroni

- Chemical reactions at very high pressure*  
Adv. Chem. Phys. **131** (2005) 105-242
- 149 L Ciabini, FA Gorelli, M Santoro, R Bini, V. Schettino V, M Mezouar  
*High-pressure and high-temperature equation of state and phase diagram of solid benzene*  
Phys. Rev. B **72** (2005) 094108
- 150 M Citroni, M Ceppatelli, R. Bini, V Schettino  
*High-pressure reactivity of propene*  
J. Chem. Phys. **123** (2005) 194510
- 151 Marco Pagliai, Marcella Iannuzzi, Gianni Cardini, Michele Parrinello, Vincenzo Schettino  
*Lithium hydroxide phase transition under high pressure: an ab initio molecular dynamics study*  
Chem. Phys. Chem. **7** (2006) 141-147
- 152 Marco Pagliai, Luca Bellucci, Maurizio Muniz-Miranda, Gianni Cardini, Vincenzo Schettino  
*A combined Raman, DFT and MD study of the solvation dynamics and the adsorption process of pyridine in silver hydrosols*  
Phys. Chem. Chem. Phys. **8** (2005) 171-178
- 153 A. Barducci, R. Chelli, P. Procacci, V. Schettino, F. L. Gervasio, M. Parrinello,  
*Metadynamics simulation of prion protein: beta-structure stability and the early stages of misfolding*  
J. Am. Chem. Soc. **128** (2006) 2705-2710
- 154 S. Marsili, A. Barducci, R. Chelli, P. Procacci, V. Schettino  
*Self-healing umbrella sampling: a non equilibrium approach for quantitative free energy calculations*  
J. Phys. Chem. B **110** (2006) 14011-14013
- 155 Elisa di Pietro, Marco Pagliai, Gianni Cardini, Vincenzo Schettino  
*Solid State Phase Transition induced by Pressure in LiOH.H<sub>2</sub>O*  
J. Phys. Chem. B **110** (2006) 13539-13546
156. Cristian Faralli, Marco Pagliai, Gianni Cardini, Vincenzo Schettino,  
*Structure and dynamics of Br<sup>-</sup> ion in liquid methanol*  
J. Phys. Chem. B **110** (2006) 14923-14928
- 157M. Pagliai, C. Cavazzoni, G. Cardini, G. Erbacci, M. Parrinello, V. Schettino  
Calcolo di spettri vibrazionali di cristalli da principi primi  
Notizie dal CINECA 2007
- 158 Gianni Cardini, Maurizio Muniz-Miranda, Marco Pagliai and Vincenzo Schettino  
*A density functional study of the SERS spectra of pyridine adsorbed on silver clusters*  
Theor. Chem. Acc. **117** (2007) 451-458
- 159 Maurizio Muniz-Miranda, Gianni Cardini, Marco Pagliai and Vincenzo Schettino  
*DFT investigation on the SERS band at ~1025 cm<sup>-1</sup> of pyridine adsorbed on silver*  
Chem. Phys. Lett. **436** (2007) 179-183
- 160 V. Schettino, R. Chelli, S. Marsili, A. Barducci, C. Faralli, M. Pagliai, P. Procacci, G. Cardini  
*Problems in molecular dynamics of condensed phases*  
Theor. Chem. Acc. **117** (2007) 1105-1120
- 161 L. Ciabini, F. A Gorelli, M. Santoro, Roberto Bini, V. Schettino, S. Raugei  
*Triggering dynamics of the high-pressure benzene amorphization*  
Nature Mater. **6** (2007) 39-43
- 162 M Citroni, M Ceppatelli, R. Bini, V Schettino  
*Dimerization and polymerization of isoprene at high pressures*  
J. Phys. Chem. B **111** (2007) 3910-3917
- 163 Roberto Bini, Vincenzo Schettino  
*Constraining molecules at the closest approach: chemistry at high pressure*  
Chem. Soc. Rev. **36** (2007) 869-880
- 164 Cristian Faralli, Marco Pagliai, Gianni Cardini, Vincenzo Schettino  
*The solvation dynamics of Na<sup>+</sup> and K<sup>+</sup> ions in liquid methanol*  
Theor. Chem. Acc. **118** (2007) 417-423

- 165 Elisa di Pietro, Gianni Cardini, Vincenzo Schettino  
*Ab Initio Molecular Dynamics Study of the Hydrolysis Reaction of Diborane*  
Phys. Chem. Chem. Phys. **9** (2007) 3857-3863
- 166 Vincenzo Schettino, Marco Pagliai, Gianni Cardini  
*Molecular dynamics of chemical reactions and phase transitions at high pressure*  
Chem. Today **25** (2007) 82- 84
- 167 G. Nannucci, L. Moroni, C. Gellini, R. Chelli, P.R. Salvi V. Schettino and G. Dellepiane  
*Fluorescence emission and torsional conformations in pi-conjugated chains of polyDCHD-HS*  
J.Phys. Chem. C **111** (2007) 17485-17492
- 168 M. Mugnai, G. Cardini, V. Schettino and C.J. Nielsen  
*Ab initio molecular dynamics study of aqueous formaldehyde and methanediol*  
Mol.Phys. 105 (2007) 2203-221
- 169 C. Faralli, M. Pagliai, G. Cardini and V. Schettino  
*Ab initio molecular dynamics study of Mg<sup>2+</sup> and Ca<sup>2+</sup> in liquid methanoli*  
J. Chem Theory Comput. 4 (2008) 156-163
- 170 M. Muniz-Miranda, M. Pagliai, G. Cardini, L. Messori, B. Bruni, A. Casini M. Di Vaira and V. Schettino  
*A multi-technique approach to predicting the molecular structure of cuprizone in the gas phase and in the cristalline state.*  
CrystEngComm, XX (2008)1-8
- 171 M. Muniz-Miranda, M. Pagliai, G. Cardini and V. Schettino  
*The role of surface metal clusters in the SERS spectra of ligands adsorbed on Ag colloidal particles*  
J. Phys. Chem. C. 112 (2008) 762-767
- 172 Simone Marsili, Riccardo Chelli, Vincenzo Schettino and Piero Procacci  
*Thermodynamics of stacking interactions in proteins*  
PCCP 10 (2008) 2673-2685
- 173 Marco Pagliai, Carlo Cavazzoni, Gianni Cardini, Giovanni Erbacci, Michele Parrinello and Vincenzo Schettino  
*Anharmonic infrared and Raman spectra in the Car-Parrinello molecular dynamics simulation.*  
J. Chem. Phys., **128** (2008) 224514-7
- 174 Martina Mugnai, Marco Pagliai, Gianni Cardini and Vincenzo Schettino  
*Mechanism of the ethylene polymerization at very high pressure*  
JCTC 4 (2008) 646-651
- 175 Margherita Citroni, Frédéric Datchi, Roberto Bini, Massimo Di Vaira, Philippe Pruzan, Bernard Canny and Vincenzo Schettino  
*Crystal structure of nitromethane up to the reaction threshold pressure*  
J. Phys. Chem. B, 112 (2008) 1095-1103
- 176 Margherita Citroni, Roberto Bini, Paolo Foggi and Vincenzo Schettino  
*Role of excited electronic states in the high- pressure amorphization of benzene*  
PNAS **105** (2008) 7658-7663
- 177 Vincenzo Schettino, Roberto Bini, Matteo Ceppatelli and Margherita Citroni  
*Activation and control of chemical reactions at very high pressure*  
Physica Scripta, 78 (2008) 058104
- 178 Vincenzo Schettino, Roberto Bini, Gianni Cardini, Matteo Ceppatelli, Margherita Citroni and Marco Pagliai  
*Solid-state Transitions and Chemical Reactions at high pressure*  
Nuovo Cimento B 129 (2008) 1399-414
- 179 Vincenzo Schettino, Roberto Bini, Matteo Ceppatelli and Margherita Citroni  
*Spectroscopic monitoring of high pressure phenomena.*  
Mol. Struct. 924-26 (2009) 2-8

- 180 Matteo Ceppatelli, Roberto Bini, Vincenzo Schettino  
High pressure photodissociation of water: a tool for hydrogen synthesis and fundamental chemistry  
PNAS 106 (2009) 11454-59
- 181 Margherita Citroni, B. Costantini Roberto Bini, Vincenzo Schettino  
Crystalline indole at high pressure: Chemical stability, electronic and vibrational properties  
J. Phys. Chem. B 113 (2009) 13526-36
- 182 Marco Pagliai, Maurizio Muniz-Miranda, Gianni Cardini, Vincenzo Schettino  
Solvation dynamics and adsorption on Ag hydrosols of oxazole: a Raman and computational study  
J. Phys. Chem. A 113 (2009) 15198-205
- 183 Matteo Ceppatelli, Roberto Bini, Vincenzo Schettino  
High pressure reactivity of model hydrocarbons driven by Near UV photodissociation of water  
J. Phys. Chem. B 113 (2009) 14640-47
- 184 Margherita Citroni, Roberto Bini, Marco Pagliai, Gianni Cardini, Vincenzo Schettino  
*Nitromethane Decomposition under High Static Pressure*  
J. Phys. Chem. B, **114** (2010) 9420-9428
- 185 M. Muniz-Miranda, C. Gellini, M. Pagliai, M. Innocenti, P.R. Salvi, V. Schettino  
SERS and Computational Studies on MicroRNA Chains Adsorbed on Silver Surfaces  
J. Phys. Chem. C., **114** (2010) 13730-13735
- 186 Marco Pagliai, Francesco Muniz-Miranda, Gianni Cardini, Roberto Righini, and Vincenzo Schettino,  
*Hydrogen Bond Dynamics of Methyl Acetate in Methanol*  
J. Phys. Chem. Letters, **1** (2010) 2951-2955
- 187 Matteo Ceppatelli, Roberto Bini and Vincenzo Schettino  
*High-pressure reactivity of clathrate hydrates by two-photon dissociation of water*  
PCCP **11** (2010) 1-12
- 188 Maurizio Muniz-Miranda, Cristina Gellini, Pier Remigio Salvi, Vincenzo Schettino, Marco Pagliai, Massimo Innocenti  
Nanostructured Ag Platforms as Biosensors of Nucleobase Chains  
J. Nanosci. Nanotechnol., **11** (2011) 1-5
- 189 Marco Pagliai, Maurizio Muniz Miranda, Gianni Cardini and Vincenzo Schettino  
*Raman and infrared spectra of minerals from ab initio molecular dynamics simulations: the spodumene crystal*  
J. Mol. Structure **993** (2011) 151-154
- 190 Francesco Muniz Miranda, Marco Pagliai, Gianni Cardini and Vincenzo Schettino  
*Wavelet transform for spectroscopic analysis: an application to simple diols in heavy water*  
J. Phys. Chem. B **7** (2011) 1109-1118
- 191 M.Pagliai; F.Muniz-Miranda; G.Cardini; R.Righini; V.Schettino  
Spectroscopic properties with a combined approach of ab initio molecular dynamics and wavelet analysis  
J. Mol Struct. **993** (2011) 438-442
- 192 F.Muniz-Miranda; M.Pagliai; G. Cardini; V.Schettino  
Spectroscopic properties of hydrogen-bonded systems by wavelet analysis.  
EUCMOS - 30th European Congress of Molecular Spectroscopy, Firenze, EUCMOS, pp. 251-251.
- 193 M. Pagliai; F.Muniz-Miranda; G.Cardini; R.Righini; V. Schettino  
Hydrogen bond dynamics of methyl acetate in methanol.  
30th European Congress of Molecular Spectroscopy, Firenze, 2010, p. 271
- 194 M. Pagliai; S. Caporali; M. Muniz-Miranda; G. Pratesi; V. Schettino  
SERS, XPS, and DFT Study of Adenine Adsorption on Silver and Gold Surfaces.  
J. Phys. Chem. Letters **3** (2012).242-245
- 195 S. Caporali; V. Moggi-Cecchi; M. Muniz-Miranda; M. Pagliai; G. Pratesi; V. Schettino  
SERS investigation of possible extraterrestrial life traces: Experimental adsorption of adenine on a Martian meteorite  
Meteoritic & Planetary Science **47**, (2012), 853-860
- 196 S. Caporali, V. Moggi-Cecchi, M. Muniz-Miranda, M. Pagliai, G. Pratesi, V. Schettino

- Surface-Enhanced Raman Micro-Spectroscopy of Adenine Adsorbed on Martian Meteorite as a Test for a Search of Extraterrestrial Life Traces  
42nd Lunar and Planetary Science Conference, The Woodlands, Texas, March, 2011, Lunar and Planetary Institute, vol. 42, pp. 1401197
- 197 S. Caporali; M. Pagliai; G. Pratesi; V. Schettino  
Surface-enhanced Raman scattering investigation of nucleobases adsorbed on samples of Martian analogue material  
Spectroscopy Letters 44 (2011) 580-584
- 198 S. Caporali; V. Moggi-Cecchi; M. Muniz-Miranda; M. Pagliai; G. Pratesi; V. Schettino  
Adenine Adsorbed on a Martian Meteorite as a Test Case for SERS Investigation of Extraterrestrial Life Trace  
Conference on Micro-Raman Spectroscopy and Luminescence Studies in the Earth and Planetary Sciences, Madrid 2011 p. 4041
- 199 Maurizio Muniz-Miranda, Marco Pagliai, Francesco Muniz-Miranda and Vincenzo Schettino  
Raman and Computational study of solvation and chemisorption of thiazole in Silver Hydrosol  
Chem. Commun. 47 (2011) 3138-3140
- 200 M. Muniz-Miranda; C. Gellini; P. R. Salvi; M. Innocenti; M. Pagliai; V. Schettino  
Fabrication of nanostructured silver substrates for surface-enhanced Raman spectroscopy.  
J. Nanoparticle Research, 13 (2011) 5863-5871
- 201 M. Pagliai; F. Muniz Miranda; V. Schettino; M. Muniz-Miranda  
Competitive Solvation and Chemisorption in Silver Colloidal Suspensions  
UK Colloids 2011, Springer, vol. 139, pp. 39-44
- 202 M. Pagliai; M. Muniz-Miranda; G. Cardini; V. Schettino  
Raman and infrared spectra of minerals from ab initio molecular dynamics simulations: The spodumene crystal  
J. Mol. Struct. 993 (2011) 151-154
- 203 R. Bini; M. Ceppatelli; M. Citroni; V. Schettino  
From simple to complex and backwards. Chemical reactions under very high pressure  
Chem. Phys. 398 (2012) 262-268
- 204 G. Cardini; V. Schettino  
Comment on "Fermi resonance in solid CO<sub>2</sub> under pressure" [J. Chem. Phys. 138, 074501 (2013)].  
J. Chem. Phys. 140, (2014) 177101-177101
- 205 Pagliai, Marco; Cammi, Roberto; Cardini, Gianni; Schettino, Vincenzo  
XP-PCM Calculations of High Pressure Structural and Vibrational Properties of P4S3  
J. Phys. Chem. A 120 (2016) 5136-5144
- 206 Caratelli, C.; Cammi, R.; Chelli, R.; Pagliai, M.; Cardini, G.; Schettino, V.  
Insights on the Realgar Crystal Under Pressure from XP-PCM and Periodic Model Calculations  
J. Chem. Phys. A 121 (2017) 8825-8834
- 207 Pagliai, M.; Osticioli, I.; Nevin, A.; Siano, S.; Cardini, G.; Schettino, V.  
DFT calculations of the IR and Raman spectra of anthraquinone dyes and lakes  
J. Raman Spectr. 49 (2018) 668-683
- 208 Bocalini M.; Cammi R.; Pagliai M.; Cardini G.; Schettino V.  
Toward an Understanding of the Pressure Effect on the Intramolecular Vibrational Frequencies of Sulfur Hexafluoride  
J. Phys. Chem. A 125 (2021) 6362-6373

## **LIBRI**

1. Vincenzo Schettino  
*Le vibrazioni delle molecole*  
Sansoni, Firenze (1975)
2. Salvatore Califano, Vincenzo Schettino, Natale Neto  
*Lattice Dynamics of Molecular Crystals*  
Springer-Verlag **26** (1981)
3. Roberto Bini, Vincenzo Schettino *Materials under extreme conditions. Molecular crystals at high pressure*  
Imperial College Press, 2013
4. Vincenzo Schettino  
*Scienza e arte. Chimica, arti figurative e letteratura*  
FUP Firenze 2014
5. Vincenzo Schettino  
*La decima musa. Poesia e scienza,*  
FUP Firenze 2016
6. Salvatore Califano e Vincenzo Schettino  
*La nascita della meccanica quantistica,*  
FUP Firenze 2018
7. Vincenzo Schettino  
*Mondi Inesplorati. La materia in condizioni estreme.*  
Bardi Roma 2024
8. Salvatore Califano, Vincenzo Schettino  
*L'atomo: una storia millenaria,*  
Fup Firenze 2024

## **ALTRE PUBBLICAZIONI**

1. Vincenzo Schettino  
*Cristalli molecolari*  
in *Enciclopedia della Fisica* , ISEDI (1976) 111-125
2. Vincenzo Schettino  
*Infrared and Raman spectra of molecular crystals: lattice dynamics and intermolecular forces*  
*Giornate Italiane della Scienza Budapest 1980*
3. Franco Bogani, Gianni Cardini, Vincenzo Schettino and Pier Luigi Tasselli  
*Dynamics of two-phonon bound states: calculation of three- and four-phonon Green functions*  
Dept. of physics, University of Florence, Internal Report **113** (1989)
4. Vincenzo Schettino  
*La ricerca Chimica in Toscana*  
Istituzioni Culturali in Toscana (2000)
5. Vincenzo Schettino  
*Le simmetrie nel mondo delle molecole*  
*Le Scienze* (2001) 78-83
6. Vincenzo Schettino, Martina Mugnai  
*Quantum mechanics: Molecules*  
In *Encyclopedia of condensed matter physics* (2004)
7. Vincenzo Schettino  
*Le scienze sperimentali ed esatte nell'Ateneo Fiorentino*  
in *L'UNIVERSITA' DEGLI STUDI DI FIRENZE 1924-2004*, Olschki, Firenze 2004

- 8 Vincenzo Schettino  
*Il Polo Scientifico di Sesto Fiorentino*  
in UNIVERSITA' E TERRITORIO, a cura di S. Rogari, Florence University Press, 2006
- 9 Vincenzo Schettino  
*Alcune riflessioni sui concorsi universitari*  
Chimica e Industria, **77** (1995) 79-80
- 10 – Salvatore Califano e Vincenzo Schettino  
*A.L. Lavoisier: Traité Élémentaire de Chimie* 163-197  
In *Là dove il pensiero incontra l'esperienza*, A.N. Neri Ed. Edizioni ETS 2017
- 11 Vincenzo Schettino  
*Ugo Schiff e la scienza in Toscana nel secondo '800*  
*Atti e memorie dell'Accademia toscana di scienze e lettere La Colombaria : volume LXXXII ; nuova serie. Vol. 68, Anno 2017 , 303-320*
- 12 – Vincenzo schettino  
*Isaac Newton and Alchemy*  
Substantia, 1 69-76 (2017)
- 13 P.R. Salvi and V. Schettino  
*Sadi Carnot's rReflexions and the foundation of thermodynamics*
  
- 14 Vincenzo Schettino  
*Isaac Newton, professione alchimista*  
In Comics and science, 38-41 (2022)
- 15 Vincenzo Schettino  
*Science and art. Chemistry, fine arts and literature*  
*Rend. Fis. Acc. Lincei* **25**, 327–338 (2014).
- 16 Vincenzo Schettino  
*Il Sistema periodico come icona universale*  
Atti Convegni Lincei 342, Il sistema Periodico. Primo Levi Chimico e scrittore, Bardi edizioni 2022, 49-74
- 17 Vincenzo schettino  
*La diffusione della meccanica quantistica e della chimica fisica nel dopoguerra*  
In *La transizione dall'Accademia d'Italia all'Accademia dei Lincei alla Accademia dei Lincei: uno snodo nello sviluppo della chimica da Giacomo Fauser ai giorni nostri*, Bardi editore, (2024)
- 18 Vincenzo Schettino  
*Creatività nella scienza: tra sogno e realtà*  
Pegaso 220 (2024) 9-11
- 19 M. Pagliai, M. Muniz-Miranda, G. Cardini, V. Schettino  
*Raman and infrared spectra of minerals from ab initio molecular dynamics simulation: the spodumene crystal*  
J. Mol. Struct. 993, 151-154 (2011)
- 20 – M. Pagliai, F. Muniz-Miranda, G. Cardini, R. Righini, V. Schettino  
*Spectroscopic properties with a combined approach of ab initio molecular dynamics and wavelet analysis*  
J. Mol. Struct. 993 438-442 (2011)
- 21 – Vincenzo Schettino  
*La materia in condizioni estreme. Una chimica dell'altro mondo*  
La Chimica e l'Industria 2014 (2)
- 22 – Vincenzo Schettino



*Oro, perle smeraldi e coralli. I minerali nella farmacopea storica*

In Alimentazione, Farmaci e malattia in Toscana fra '800 e '900, E. Diana Ed. Edizioni dell'Assemblea 53-70 (2022)

23 – Elisabetta Cerbai, Vincenzo Schettino

*History and structure of the LENS*

Il Colle di Galileo, 11 45-54 (2022)