Curriculum Vitae

Prof. Cecilia Coletti

Date and place of birth: Perugia (Italy), 11/21/1969.
Nationality: Italian
Education: Degree in Chemistry at the University of Perugia (Italy) in 1993 (Supervisor Prof. Vincenzo Aquilanti); PhD in Chemical Sciences (Physical Chemistry) at the University of Perugia (Italy) in 1997 (Supervisors: Prof. Vincenzo Aquilanti and Prof. Simonetta Cavalli)
Fellowships: short-term fellowship at the University of Barcelona (Spain) with Prof. Jaime de Andres-Llopis (November 1996-February 1997); Post Doctoral Fellowship (1998-1999) at the University of Copenhagen (Denmark), H.C. Ørsted Insitute with Prof. Gert D. Billing; Post Doctoral Fellowship (December 2000-September 2001) at the University of Perugia (Prof. Simonetta Cavalli) Visiting scientist at the University of Copenhagen (Denmark), H.C. Ørsted Insitute (Prof. Gert D. Billing), with a grant of the Carlsberg Science Foundation (June 2001- August 2001)
Career: 2001-2010, Associate Researcher at the Department of Pharmaceutical Sciences, University "G. d'Annunzio", Chieti-Pescara (Italy); 2010-present, Associate Professor at the Department of Pharmacy, University "G. d'Annunzio", Chieti-Pescara (Italy)
Memberships: Italian Chemical Society (SCI), American Chemical Society (ACS)

Scientific Activity: The activity of Prof. Cecilia Coletti is mainly devoted to the theoretical investigation of molecular structure and dynamics starting from model systems, through systems of growing complexity, to macromolecules of biological and pharmaceutical interest. She has worked with Prof. Aquilanti (University of Perugia) and Prof. J. Avery (University of Copenhagen) on the development of alternative coordinate systems and basis sets to be used for the description of atomic structures or for atoms in fields. Working with Prof. G. Billing, she addressed the detailed description of the nuclear dynamics of molecular systems, contributing to the development of novel mixed quantum-classical methodologies and to their application to systems of interest in atmospherical, optical and laser chemistry. More recently, at the University of Chieti, her reserach inter-

ests focus on the accurate investigation of simple systems or of weak interactions using highly correlated post Hartree-Fock methods and on the study of the electronic structure, binding and reactivity of organometallic compounds of technological and pharmaceutical importance, by quantum mechanical techniques (DFT, post-HF methods), QM/MM or molecular modeling.
This activity is reported in ca. 60 papers published on international journals and reviews and the results have been presented in more than 100 international workshops and conferences.
Peer reviewer for the Journal of Physical Chemistry A, Chemical Physics, Chemical Physics Letters, Physical Chemistry Chemical Physics, Theoretical Chemistry Accounts, Molecular Physics, Journal of Computational Chemistry, Applied Catalysis B, Zeitschrift für Naturforchung A, Journal of Organometallic Chemistry, etc.
Coeditor of a Special Issue of the Journal of Physical Chemistry (2003).

Teaching Activity: "General and Inorganic Chemistry" (2002-present) at the Department of Pharmacy (University of Chieti); "Computational Chemistry" (2004-present) at the Department of Pharmacy (University of Chieti)

Publications

1. V. Aquilanti, S. Cavalli, C. Coletti, D. De Fazio, G. Grossi
"Hyperangular Momentum: Applications to Atomic and Molecular Science"
in *New Methods in Quantum Theory*, *C.A. Tsipis, V.S. Popov, D.R. Herschbach, J.S. Avery Eds.*, Kluwer, (1996); 233-250

2. V. Aquilanti, S. Cavalli, C. Coletti, G. Grossi
"Alternative Sturmian Bases and Momentum Space Orbitals: an Application to the Hydrogen Molecular Ion"
Chem. Phys., **209** (1996), 405-419

3. V. Aquilanti, S. Cavalli, C. Coletti
"The d-dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals and alternative Sturmian basis sets."
Chem. Phys., **214** (1997), 1-13

4. V. Aquilanti, S. Cavalli, C. Coletti
"Hyperspherical Symmetry of Hydrogenic Orbitals and Recoupling Coefficients among Alternative Bases"
Phys. Rev. Lett., **80** (1998), 3209-3212

5. C. Coletti and G.D. Billing
"Isotopic effects on vibrational energy transfer in CO"
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6. C. Coletti and G.D. Billing
"Reaction-volum approach to N-particle reactions: New optimization scheme for defining the reaction volume"
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7. V. Aquilanti, S. Cavalli, C. Coletti, D. Di Domenico and G. Grossi
"Hyperspherical Harmonics as Atomic and Molecular Orbitals in Momentum Space"
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8. C. Coletti and G.D. Billing
"Quantum-classical methods: a quantum-classical approach to diatom-diatom reactive scattering and VV energy transfer"
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9. J. Avery and C. Coletti
"Many-electron Sturmians applied to atom and ions in strong external fields"
"New Trends in Quantum Systems in Chemistry and Physics. Vol. I", J. Maruani et al. Eds. (Kluwer Academic Publishers), (2001): 77-93

10. J. Avery and C. Coletti
"Generalized Sturmians Applied to atoms in strong external fields"
J. Math. Chem., **27** (2000), 43-51

11. C. Coletti and G.D. Billing
"Rate constants for energy transfer in carbon monoxyde"
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12. C. Coletti and G.D. Billing
"Quantum-classical calculation of cross sections and rate constants for the H_2+CN→ HCN+H reaction"
J. Chem. Phys., **113** (2000), 11101-11108

13. C. Coletti and G.D. Billing
"Quantum dressed classical mechanics: Application to chemical reactions"
Chem. Phys. Lett., **342** (2001), 65-74

14. V. Aquilanti, S. Cavalli, C. Coletti, D. Di Domenico, G. Grossi
"Hyperspherical harmonics as Sturmian orbitals in momentum space: a systematic approach to the few-body Coulomb problem."
Int. Rev. Phys. Chem., **20**(4) (2001), 673-709

15. V. Aquilanti, S. Cavalli, C. Coletti
"Angular and Hyperangular Momentum Recoupling, Harmonic Superposition and Racah Polynomials. A recursive algorithm. "
Chem. Phys. Lett., **344** (2001), 587-600

16. V. Aquilanti and C. Coletti
"3nj-symbols and harmonic superposition coefficients: an icosahedral abacus "
Chem. Phys. Lett., **344** (2001), 601-611

17. C. Coletti
"Vibrational energy transfer in diatomic collisions: A mixed quantum classical approach"
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18. C. Coletti and G.D. Billing
"Vibrational energy transfer in molecular oxygen collisions"
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19. V. Aquilanti, A. Caligiana, S. Cavalli and C. Coletti
"Hydrogenic Orbitals in Momentum Space and Hyperspherical Harmonics. Elliptic Sturmian Basis Sets"
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20. G.D. Billing, C. Coletti, A.K. Kurnosov and A.P. Napartovich
"Sensitivity of molecular vibrational dynamics to energy exchange rate constants"
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21. C. Coletti and G.D. Billing
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22. A. Marrone, C. Coletti, N. Re
"Metal Fragment Modulation of Metallacumulene Complexes: A Density Functional Study"
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23. M. Baer, C. Coletti, G. C. Schatz, S. Toxvaerd, L. Wang
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24. D. Bellocchi, G. Costantino, R. Pellicciari, N. Re, A. Marrone, C. Coletti
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25. C. Coletti and N. Re
"Theoretical study of alkali cation-benzene complexes: Potential energy surfaces and binding energies with improved results for rubidium and cesium"
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45. C. Coletti, N. Re
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"Theoretical determination of the microstructure of Cs covering of Mo in negative ion sources for nuclear fusion applications"
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