Dr. Giorgio F. Signorini
Curriculum Vitae

Name: Giorgio Federico Signorini

Born: 21/02/1959 Firenze (Italy)

Citizenship: Italian

Marital status: married (1998), one child (born 2004)

Address: Dipartimento di Chimica, Università di Firenze
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EDUCATION

High School: Liceo Classico "Dante", Firenze (1973-1978)

University: Degree in Chemistry, Università di Firenze (1979-1985)
Final mark: 110/110 *cum laude*
Dissertation in Molecular Spectroscopy: *"Lattice Dynamics and Anharmonic Processes in Molecular Crystals: Anthracene and Nitrogen"* (Supervisor: Prof. V. Schettino)

Ph. D.: Dottorato di Ricerca in Scienze Chimiche, curriculum Chimica Fisica dello Stato Solido (Physical Chemistry of Solid State) (1986-1989)
Dissertation: *"Dynamical Properties and Relaxation Processes in Condensed Molecular Systems"*

EMPLOYMENT

- Post-Doctoral Fellow at the University of Pennsylvania, Philadelphia, USA; Prof. Michael L. Klein (1989-1990)
- IBM Study Contract with Università di Firenze: *"Connection of different computing systems through token-ring and Portability of Unix applications"* (1990-1991)
- Member of Scientific-Technical staff, Dipartimento di Chimica, Università di Firenze (1991-present)

RESEARCH FIELDS

intermolecular potentials: models for intermolecular potentials and their use in computational schemes such as Molecular Dynamics (MD) and Lattice Dynamics (LD); transferable force fields; influence of different parts of potential on anharmonicity; simulation of crystal-liquid transition

vibrational states of molecular crystals: harmonic and anharmonic LD of molecular crystals; extension of standard LD treatment to crystals of molecular ions; relaxation processes of internal and external phonons, vibrational band broadening; approximate computation of high-order contributions to bandwidth; temperature and pressure effect on bandwidths; contribution of orientational disorder to bandwidths: MD simulations and comparison to LD;

spectroscopic properties of impurities: vibrational relaxation of a doping molecule in a host molecular lattice; pressure dependence of vibronic band frequencies of a small molecule in a rare-gas matrix;

dynamics of molecular liquids: structure and structure relaxation near the glass transition; comparison of simulation results to predictions of mode-coupling theory; relaxation of rotational degrees of freedom

advanced simulation methods: application of nonequilibrium simulations for the computation of free energy differences; generalized ensemble methods (Replica Exchange, Serial Generalized Ensemble, etc.)

OTHER PROFESSIONAL INTERESTS

archaeometry: non-destructive spectroscopic analysis of painting materials from rock art sites

computer systems and networks: IBM VM/CMS mainframe computer and UNIX workstation administration; TCP/IP network design and administration; DNS server administration; electronic mail management

Open Source and sustainable_development: the "Open Source" model applied to fields other than software; shared knowledge and development; open access publication, open science, open education

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TEACHING EXPERIENCES

- *Fortran Programming,* for Chemistry students, Università di Firenze, 1990/91
- *The VM/CMS operating system,* cycle of lessons and lab sessions for Theoretical Chemistry students, Università di Firenze, 1990/91
- *Lattice Dynamics calculations on Ionic Crystals*, seminar for Solid State Physical Chemistry students, Università di Firenze, 1994/95
- *Internet resources for Chemistry education,* lesson and lab session for High School teachers, Università di Firenze, 1999.
- *Molecular Dynamics Simulations,* cycle of lessons for Theoretical Chemistry students, Università di Firenze, 2000/2001 and 2001/2002.
- *Introduction to UNIX,* cycles of lessons and lab sessions in the *IT Skills* course for Chemistry students, Università di Firenze, 2001/02, 2002/03, 2003/04, 2005/06 and 2006/07
- *Introduction to the Internet,* cycles of lessons and lab sessions in the *IT Knowledge* course for students of Cultural Heritage Conservation, Università di Firenze, 2001/02, 2002/03, 2003/04, 2005/06 and 2006/07
- *Steered Molecular Dynamics Simulation of a model polypeptide,* laboratory project in the course *Structure and Dynamics of Biomolecules*, for Ph.D. students in Chemistry of Biomolecules, Università di Firenze, 2005/06
- *Monte Carlo Simulation,* laboratory project in the course *Structure and Dynamics of Biomolecules*, for Ph.D. students in Chemistry of Biomolecules, Università di Firenze, 2006/07 and 2007/08
- *Elementary Statistical Mechanics and Molecular Dynamics Simulation of proteins,* series of classes and laboratory project in the course *Structure and Dynamics of Biomolecules*, for Ph.D. students in Chemistry of Biomolecules, Università di Firenze, 2006/07
- *Elementary Statistical Mechanics* (classes), *Molecular Dynamics Simulation of proteins and advanced computational techniques for the evaluation of stability* (laboratory project); in the course *Structure and Dynamics of Biomolecules*, for Ph.D. students in Chemistry of Biomolecules, Università di Firenze, 2006/07, 2007/08, 2008/09
- *Structural Properties of Glasses* (teaching module within the course *Glasses and Ceramics*), Università di Firenze, 2013/14, 2014/15, 2015/16, 2016/17, 2017/18, 2018/19