# Maurizio Cossi

*Curriculum vitae*

## PERSONAL DATA

Born in Brescia on 1966, May 12th.
Lives in Alessandria, via De Giorgi 5.

## BIO AND EDUCATION

Professor Maurizio Cossi obtained the degree in Theoretical Chemistry in 1991 at the Scuola Normale Superiore (Pisa), where he concluded also his PhD in 1995. Since 1995 to 2001 he has been Researcher in the Department of Chemistry of the University of Naples "Federico II", since 2001 to 2006 Associate Professor of Physical Chemistry in the same Department. Since 2006, October he is Associate Professor of Physical Chemistry in the Department of Sciences and Innovation Technology (DISIT) of the Università del Piemonte Orientale.

His main research interests involve the development of theoretical models and computational algorithms for the quantum mechanical calculation of molecular properties, with a particular focus on solute-solvent interactions and on molecular layers adsorbed on conductor and semiconductor surfaces. In the field of method development, Prof. Cossi has collaborated to develop and implement one of the most diffused and known methods for the simulation of solvent effects (PCM, Polarizable Continuum Model): in particular, he has developed many algorithms for the calculation of energy derivatives and of properties in the excited states and he has produced the so-called conductor-like version of the PCM model.

Recently, he devoted to the simulation of various experimental quantities (mainly vibrational spectra, nuclear magnetic resonance and X-Ray diffrattograms) to assist and support the experimental work in joint research prjects.

Co-author of the Gaussian package (the most used quantum mechanical computational program, that is currently distributed as Gaussian09), where he gave an important contribution to the solvent effect description.

Co-author of MOLCAS program (version 7), one of the most used package for multi configurational calculations.

He has implemented a procedure for the calculation of solute-solvent interactions in periodic systems in the CRYSTAL03 program, distributed by the University of Torino to several interational research groups.

He has inserted an up-to-date model for the simulation of solvent effects in a Car-Parrinello code for molecular dynamics.

He has published 94 papers in international journals, and 4 chapters in collective books, and received more than 19000 citations. His h-index (for the evaluation of the publication impact) is currently 34 (Web of Science, May 2016).

## UNIVERSITY CAREER

| | |
|---|---|
| 1995-2001 | Researcher, Università di Napoli "Federico II" |
| 2001-2006 | Associate professor (Physical Chemistry), Università di Napoli "Federico II" |
| 2006- | Associate professor (Physical Chemistry), Università del Piemonte Orientale |

## UNIVERSITY POSITIONS

| | |
|---|---|
| 2013- | Member of the "Commissione Didattica" of the "Corsi di laurea triennale in Chimica" and "Magistrale in Scienze Chimiche" |
| 2015- | Member of the "Commissione Paritetica Docenti-Studenti (CPDS)" of Department DISIT |
| 2010-2014 | Responsible for "Piano Lauree Scientifiche" in Chemistry |
| 2015- | Responsible for "Piano Lauree Scientifiche (2015-2018)" in Chemistry |

## MAIN FIELDS OF INTEREST

1. Theoretical and computational chemistry

2. Chemical modeling

3. Nanomaterials

4. Molecule/surface interactions

5. Nanoporous solids

## CURRENT ISSUES OF RESEARCH

### 1. Theoretical and computational chemistry

Development and implementation of computational procedures for the modeling of complex chemical systems: structures, reactivity and electronic properties. In particular, concerning the simulations of environmental effects, due to solvent or solid substrates.

### 2. Modeling

Development of models for chemical systems, in order to interpret experimantal data, predict reactivity and properties, support the molecular design. Of particular importance the cooperation with experimental research groups, involved in the synthesis and characterization of new

materials. The modeling is here seen ad one of the valuable tools available to chemists for the design, synthesis and characterization of new molecules and materials.

### 3. Modeling of nanoporous solids

This is a particularly important research line in the Department: the modeling, based on procedures and parameters developed and optimized in this research group, supports the synthetic and characterization acivities, dedicated to new nanoporous materials for caprture and storage of varius gases, for energy or environmental purposes.

### 4. Modellizzazione di materiali per l'energia

This is another important research line, recently funded in various projects: the research group models several materials and processes in the photovoltaic and electrochemical fields, supporting the experimental activities.

## CURRENT FUNDED PROJECTS

| FUNDING AGENCY | ROLE | PROJECT |
|---|---|---|
| EU: 7th Framework Program | Responsible for WP1: "Benchmarking and modeling" | GLOBASOL: Global solar spectrum harvesting through highly efficient photovoltaic and thermoelectric integrated cells |
| SOL group | Responsible for theoretical modeling | Development of adsorbing materials for gas storageS |
| Fondazione San Paolo | Responsible for theoretical modeling | HEPYCHEM: Aluminophosphates with designed hierarchical porosity for green chemistry |
| Fondazione Cariplo | Local responsible | Highly Adsorptive Microporous Materials for Gas Adsorption and Storage |

## TOP FIVE PAPERS

1. Maurizio Cossi, Vincenzo Barone "Time-dependent density functional theory for molecules in liquid solutions" J. Chem. Phys. 115 (2001) 4708-4717.
2. Maurizio Cossi, Maria Francesca Iozzi, Andrea Marrani et al. "Measurement and DFT calculation of $Fe(cp)_2$ redox potential in molecular monolayers covalently bound to H-Si(100)" J. Phys. Chem. B 110(2006) 22961-22965.
3. Ilaria Braschi, Giorgio Gatti, Geo Paul, Carlo Gessa, Maurizio Cossi, Leonardo Marchese "Sulfonamide antibiotics embedded in high silica zeolite Y: A combined experimental and theoretical study of host-guest and guest-guest interactions" Langmuir 26 (2010) 9524-9532.

4. Mario Argeri, Alberto Fraccarollo, Fabio Grassi, Leonardo Marchese, Maurizio Cossi "Density functional theory modeling of PbSe nanoclusters: Effect of surface passivation on shape and composition" J. Phys. Chem. C 115 (2011) 11382-11389.

5. Alberto Fraccarollo, Lorenzo Canti, Leonardo Marchese, Maurizio Cossi "Monte Carlo modeling of carbon dioxide adsorption in porous aromatic frameworks" Langmuir 30 (2014) 4147-4156.