Maddalena D'Amore, PhD

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RESEARCH INTEREST GENERAL DESCRIPTION

The main research lies in the field of theoretical and computational chemistry of complex and large dimensions chemical systems of interest in biology and industry. During years my activity has been more and more focused on condensed matter, mainly on surface science topics and my activity has been devoted to simulations of efficient and selective catalysts and to materials for a wide range of energy and environmental applications.

The simulation of complex nanostructures with controlled crystal morphology to obtain nano-materials with a certain catalytic behavior is one between most addressed targets in material research. The aim is the identification of close relation between properties and microstructures of materials, the possibility to stabilize certain surfaces due to selective adsorption, the identification of active sites in highly performing and multisite catalysts, to fix the best thermodynamic condition of operation of materials together with the best environmental conditions to obtain new materials and improve the performances and production engineering of existing ones. In this view the development of accurate adsorption models turns to be a key topic as it is in my research activity. Theory is now moving towards the demand to provide models and describe processes with the accuracy comparable to that of finest experiments; the predictions of properties of materials and the design of heterogeneous catalysts is becoming feasible this thanks to recent advances in Density Functional Theory. Hence I have adopted computational approaches mostly based on Density Functional Theory (DFT) in order to estimate non covalent interactions, spectroscopic parameters, electric response and magnetic behavior but also a multi-scale modelling resorting to both molecular mechanics and dynamics tools can be a useful weapon. For investigated materials computation of harmonic frequencies and anharmonic corrections to those values have been also performed, in fact, when solving IR spectra, theoretical simulation can help the experimental interpretation by providing a reliable description of hydrogen bonds both in clay minerals and zeolites, significantly affecting infrared spectra the same holds true for complex catalytic systems involving bulky electron donating molecules (like benzoates or phthalates) adsorbed on supports.

My research activity stands on a synergetic cooperation between theoreticians and experimentalists (mostly spectroscopists), industrial partners are often involved, in fact I worked in Projects of the Dutch Polymer Institute (DPI, DPI Project #712) and recently the same Institution approved a project of our group on the catalysts (DPI Project PO2.0-2016-005 - DisMgCl).

In simulations I resort to both cluster models (pseudo-potentials or all-electron treatments) and periodic ones (1D, 2D and 3D periodic treatment). I' m familiar with the Quantum Mechanics Gaussian and Crystal codes based on the LCAO approach they allow the calculation of the total energy and related properties of molecules and solids (e.g. structural, electronic, vibrational, mechanical, magnetic, dielectric, etc.) at both the Hartree-Fock and DFT level, by expressing the orbitals (molecular/crystalline) in terms of a local basis set of Gaussian-type orbitals (i.e. LCAO approach). I performed *ab-initio* calculations by means of Gaussian code, thanks to the same code solvent models have been also provided. The codes have been applied to the study of many different materials with relevance in solid state chemistry, physics, materials science and catalysis.

About simulations of 'molecules' I also worked on **Parameterization of force fields** for application to nitroxide derivatives in solution for a description of large molecules of biological interest and employed AMBER code in **molecular dynamics studies**. More in detail, I was involved in the application and validation of quantum-

mechanical models to study the conformational behaviour and to determine magnetic ESR properties of nitroxide probes when introduced in peptidic systems and organic polymers both in gas phase and in condensed phase. The solvent effects on structure and magnetic properties of biomolecules have been taken into account by means of simultaneous inclusion of both bulk effects (continuum models, PCM) and specific interactions solute-solvent.

Starting with my Master thesis I collected a certain experience with **polymer science** (experimental characterizations and **Molecular Mechnics (MM**) simulations), I continued during my PhD with quantum mechanical modelling of defects in polymeric chains and physical-chemical properties of synthetic polymers of great technological interest (polyethylene, polypropylene, Teflon). I also simulated electronic properties of conductive polymers (polythiophenes) and their electric field response.

A further valuable experience bound to macromolecules concerns the simulation of **heterogeneous catalysts** it has been gained first, through the modeling of geometry, electronic structure and magnetism of α, β and γ forms of the progenitor $TiCl_3$ catalyst and then by the study of fourth generation $MgCl_2$-supported Ziegler-Natta catalysts for α-olefin polymerization. In these cases special attention has been devoted to a first evaluation of Van der Waals forces, these brought to significantly new insights in the comprehension of these catalysts. To describe the long-range electron correlations responsible for Van der Waals forces two basic strategies have been considered and each of them is being used more and more in surface science and to address solid state problems. One entails a classical correction (of the type $f(R)/R^6$) to the DFT energies and gradients, namely the DFTD method; the other strategy consists in the adoption of one of the last-generation highly parametrized forms of hybrid meta-GGA DF's, namely the M06 exchange-correlation functional suite.

In the framework of the **study of chemical bonding** in complex metal-ligands systems, I was recently involved in the development and applications of bond analysis in both molecules and crystals as models relevant to bio-inorganic chemistry by the recent Maximum Probability Domains (**MPD**) and Electron Localization Function (**ELF**) analyses. I'm involved in the validation of CRYSTAL code, in particular of tools predicting morphology and defective positions in crystals ("edge", "rods", nanocrystals) and of the above mentioned chemical bond analysis through ELF e MPD.

I'm working to build models for capture, storage and activation of CO_2 by recently designed materials, "Metal-Organic Framework (**MOF**)" are between them, I studied the structure and reactivity of adsorption sites in the giant MIL-100 and in CuBtc similarly I'm currently investigating CO_2 adsorption on MgO clusters enclosed in a Y zeolite.

Nowadays thanks to recent evolutions in High Performance Computing (HPC) architectures and the concurrent development of more efficient quantum-mechanical software have already shown the possibility to increase the size and complexity of the systems that can be tackled by quantum mechanical methods. I'm validating a highly massive parallel (MPP) version of CRYSTAL is available on HPC resources that has been specifically tailored to achieve an excellent scalability in terms of both speed-up and memory usage to make computation possible on investigated nanosystems About HPC resources access, I obtained two ISCRA C projects at CINECA: POLCAT (Modeling heterogeneous Ziegler-Natta catalysts for olefin conversion) and SASP (Simulation of Active sites of Polimerization) at CINECA (Italy), and projects at the Abel facility at the University of Oslo (Norway); I'm also a co-investigator in an ISCRA C project on astrochemistry with Prof. V. Barone as principal investigator..

At this very moment **I'm** the **Principal Investigator** of a **PRACE (**Partnership for Advanced Computing in Europe) **project** titled "Modelling mechanism of reactions and active sites in Ziegler-Natta nano-systems, looking for reactivity indicators in heterogeneous catalysis" (proposal number 2016163997). In PRACE Call 15 for Project Access the Proposal 2016163997 is amongst those being awarded resources: the amount of resources allocated to my project is 30,0 million core hours on SuperMUC computing platform (GCS/LRZ, Germany), for a period of 12 months. The present project has been approved in the PRACE Call 15 with the highest score by three reviewers.

PERSONAL INFORMATION

Name: Maddalena D'Amore **Gender:** Female

Current Location: Torino, Italy. **Nationality:** Italian

CURRENT ROLE

Since May 2014 Post Doc position at Department of Chemistry of University of Torino.

1 August 2017 up to now working on the project "*Ab-initio* computational study of $MgCl_2$ and $MgCl_2/TiCl_4$ Ziegler-Natta catalysts". Scientific leader: Prof. Bartolomeo Civalleri. Also involved in a Dutch Polymer Institute (DPI) Project PO2.0-2016-005 – DisMgCl with Prof. Elena Groppo.

SOME PREVIOUS EXPERIENCES

06/2016 - 06/2017 **Post-doc fellowship.**

- Research Project "Modeling heterogeneous Ziegler Natta catalysts for olefin conversion". The scientific leader is Prof. Elena Clara Groppo, I work in the group of Prof. S. Bordiga in cooperation with Department of Chemical, Materials and Production Engineering of University of Naples "Federico II".

01/03/2016 - 31/05/2016 **Grant of Department of Chemical, Materials and Production Engineering of University of Naples Federico II, Napoli**

- working on Project PON_03PE_0111_1 "MATEMI" under the guidance of Prof. Giuseppe Mensitieri**.**

05/2014 - 05/2015 **Fellowship of Department of Chemistry of University of Torino (Theoretical Chemistry Group)**

- working on a PRACE Project (PRACE Grant: Project 2013081680) of Prof. B. Civalleri and in cooperation with Prof. M. Causà at Department of Chemical, Materials and Production Engineering of University of Naples Federico II, Napoli. The SUPERMUC "petascale system" was employed. The research Project was titled "*Ab initio* study of capture and storage of CO_2 in hybrid microporous materials".

05/2009 - 05/2014 **Post Doc, University of Napoli, "Federico II" (Group of Prof. V. Busico)**

- In charge of a research project of Dutch Polymer Institute titled "Elucidation and control of the active surface structure and chemistry in $MgCl_2$-supported Ziegler-Natta catalysis: an integrated experimental and computational approach". The project was developed in cooperation with Eindhoven University of Technology (TU/E) and Japan Advanced Institute of Science and Technology (JAIST).
- Research subject: "Theoretical computation on systems donor-spacer-acceptor".

01/2005 - 04/2005 **Fellowship of Department of Chemistry, University of Napoli, "Federico II", Group of Prof. V. Barone;**

- Research subject: " Macromolecules in nano-organized structures".

05/2004- 09/2004 **Research scholar at the "Center for nanoscale science and technology" Rice University, Houston–Texas, in the group of prof. G. Scuseria at Gaussian Inc.**

- Research subject: Gaussian code for periodic system.

Publications

1. M. D' Amore, R. Improta, V. Barone, "Conformational Behavior and Magnetic Properties of a Nitroxide Amino Acid Derivative in Vacuo and in Aqueous Solution", *Journal of Physical Chemistry A* **2003**, 107, 6264-6269.
2. M. D' Amore, F. Auriemma, C. De Rosa, V. Barone, "Disordered Chain Conformations of Polytetrafluoroethylene in the High Temperature Crystalline Form I", *Macromolecules* **2004**, 37, 9473-9480.
3. M. D' Amore, G. Talarico and V. Barone, "Periodic and High-Temperature Disordered Conformation of Polytetrafluoroethylene Chains: an Ab-Initio Modelling", *Journal of American Chemical Society* **2006**,128(4); 1099-1108.

4. M. D' Amore, C. Bisio, G. Talarico, M. Cossi, L. Marchese, "The Interface between Alkylammonium Ions and Layered Aluminophosphates Materials: A Combined Theoretical and Experimental Study", *Chemistry of Materials* **2008**, 20, 4980–4985.
5. L. Sementa, M. D 'Amore, V. Barone, V. Busico, V., M. Causa', "A Quantum Mechanical Study of α, β and γ Crystal Phases of TiCl3: Geometry, Electronic Structure and Magnetism", *Phys. Chem. Chem. Phys*., **2009**, 11, 11264-11275.
6. M. D' Amore, R. Credendino, P. H. M. Budzelaar, M. Causá, V. Busico, "A Periodic Hybrid DFT Approach (Including Dispersion) to $MgCl_2$-Supported Ziegler-Natta Catalysts, 1. $TiCl_4$ Adsorption on $MgCl_2$ Crystal Surfaces", *Journal of Catalysis*, **2012**, 286, 103-110.
7. P. Caruso, M. Causa', P. Cimino a, O. Crescenzi, M. D' Amore, R. Improta, N. Rega: "Effects of Molecular Dynamics and Solvation on the Electronic Structure of Molecular Probes, *Theoretical Chemistry Accounts*, **2012**, 131, 1-12.
8. M. Causà, M. D' Amore, C. Garzillo, F. Gentile and A. Savin, "The Bond Analysis Techniques (ELF and Maximum Probability Domains) Application to a Family of Models Relevant to Bio-Inorganic Chemistry", in "Applications of Density Functional Theory to Biological and Bioinorganic Chemistry". Series: Structure and Bonding, Vol. 150, Putz, Mihai V.; Mingos, D. Michael P. (Eds.), DOI: 10.1007/978-3-642-32750-6_4, ISBN 978-3-642-32749-0, Springer-Verlag Berlin Heidelberg 2013.
9. M. Fusaro, V. Barone, M. Causà, M. D' Amore, C. Garzillo, "Theoretical Analysis of the Reactivity of Carbon Nanotubes: Local versus Topological Effects", in "Topological Modelling of Nanostructures and Extended Systems", Ashrafi, A.R.; Cataldo, F.; Iranmanesh, A.; Ori, O (Editors); Springer Science + Business Media Dordrecht 2013.
10. F. Capone, L. Rongo, M. D' Amore, P. H. M. Budzelaar, V. Busico, "A Periodic Hybrid DFT Approach (Including Dispersion) to $MgCl_2$-Supported Ziegler-Natta Catalysts: 2. Model Electron Donor Adsorption on $MgCl_2$ Crystal Surfaces", *Journal of Physical Chemistry C*, **2013**, 117 (46), 24345-24353 .
11. M. Causà, M. D' Amore, F. Gentile, M. Menendez, M. Catalayud, "Electron Localization Function and Maximum Probability Domains analysis of semi-ionic oxides crystals, surfaces and surface defects", *Computational and theoretical Chemistry* **2015**, 1053, pp. 315-321.
12. E. Morra, Prof. E. Giamello, Prof. S. Van Doorslaer, G. Antinucci, Dr. M. D' Amore, Prof. V. Busico and Prof. M. Chiesa, "Probing the Coordinative Unsaturation and Local Environment of Ti^{3+} Sites in an Activated High-Yield Ziegler–Natta Catalyst", *Angewandte Chemie* **2015**, 54 (16), 4857-4860.
13. M. D'Amore, Thushara K.S., A. Piovano, M. Causà, S. Bordiga, E. Groppo, " Surface Investigation And Nanoscale Morphological Analysis Of Coordinatively Unsaturated Surfaces In Structurally Disordered MgCl2 And MgCl2/TiCl4 Ziegler-Natta Catalysts", *ACS Catalysis*, **2016**, 6, 5786-5796.
14. K. S. Thushara, M. D' Amore, A. Piovano, S. Bordiga, E. Groppo, " The influence of alcohols in driving the morphology of $MgCl_2$ nanocrystals", *Chem.Cat. Chem.* **2017**, 9, 1782-1787.
15. A. Piovano, M. D' Amore, K. S. Thushara, E. Groppo, "Spectroscopic evidences tor $TiCl_4$/donor complexes on the surface of $MgCl_2$-supported Ziegler-Natta catalysts", *Journal of Physical Chemistry C,* **2018***,* 122, 5615-5626*.*
16. T. Fornaro, J. R. Brucato, C. Feuillie, D.A. Sverjensky, R. M. Hazen, R. Brunetto, M. D'Amore, V. Barone, "Binding of Nucleic Acid Components to the Serpentinite-Hosted Hydrothermal Mineral Brucite", *Astrobiology*, **2018**, 18(8), ast.2017.1784. https://doi.org/10.1089/ast.2017.1784.
17. J. G. Vitillo, T. Fjermestad, M. D'Amore, M. Milanesio, L. Palin, G. Ricchiardi and S. Bordiga, "On the structure of superbasic (MgO)n sites solvated in a faujasite zeolite", *Phys. Chem. Chem. Phys.*, **2018**, 20, 18503.
18. S. Salustro, F. Colasuonno, A.M. Ferrari, M. D' Amore, W. C. Mackrodt, R. Dovesi, "Substitutional boron and nitrogen pairs in diamond. A quantum mechanical vibrational analysis", *Carbon* **2019**, 146, 709-716. https://doi.org/10.1016/j.carbon.2019.01.072.
19. M. Signorile, J. G. Vitillo, M. D' Amore, V. Crocellà, G. Ricchiardi, S. Bordiga, "Characterization and Modelling of Reversible CO_2 Capture From Wet Streams by a MgO/zeolite Y Nanocomposite", Journal of Physical Chemistry, Manuscript ID: jp-2019-01399n (under revision).