Nicolas Onofrio
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Languages: french, english

EDUCATION

Postdoc scholar — **Purdue University, West Lafayette, IN, USA**

Ph.D Computational chemistry — **University Joseph Fourier, Grenoble, FR**
Awarded September 2011 with honors
- Degree included coursework in Chemistry

M. Sc. Physical-Chemistry — **University Joseph Fourier, Grenoble, FR**
Awarded July 2008
- Degree labeled 'theoretical chemistry'

B. Sc. Physical-Chemistry — **University Joseph Fourier, Grenoble, FR**
Awarded July 2004

RESEARCH AND WORK EXPERIENCE

Postdoc
Current position

Material and Engineering, West Lafayette, IN, USA
Supervisor: Prof. Alejandro H. Strachan /strachan@purdue.edu

Title: Uncertainty quantification in multiscale modeling and surface properties of polymers

- Large scale molecular dynamic
- Uncertainties quantification

Ph.D thesis
Oct 2008 - Oct 2011

Magnetic Resonances' Laboratory at CEA, Grenoble, FR
The CEA is the French Alternative Energies and Atomic Energy Commission
Thesis Supervisor: Dr. Jean-Marie Mouesca /jean-marie.mouesca@cea.fr
Governmental grant (MRT: Research & Technology Ministry) 20 k€/year

Title: Theoretical study of the magnetic interaction in copper(II) dimers by Density Functional Theory (DFT) and Broken-Symmetry (BS) methods

Areas of expertise
- DFT (ADF code) and HF (Molcas code) computation of exchange coupling constants for copper(II) dimers and polyspin (Copper(II), radicals systems)
- Home-made Python codes: extraction of DFT parameters, representation of molecular density and formal calculations
- Molecular dynamics (Tinker code) on organic polymers (dimers and trimers)
- Analytical derivations of exchange coupling constant expressions (formal derivations vith Maxima code)

Coursework in Chemistry at University Joseph Fourier, Grenoble, FR
Tutor: Pr. Sylvain Hammam /sylvain.hamman@ujf-grenoble.fr
Governmental grant 3 k€/year for 64h/year

- Undergraduate level practical course in physical-chemistry (60h)
- Undergraduate level theoretical course in physical-chemistry (60h)
- Undergraduate level practical course in thermodynamic chemistry (30h)
- Undergraduate level practical course in inorganic chemistry (30h)

M. Sc. 2nd thesis
Jan 2008 - July 2008

Magnetic Resonances' Laboratory at CEA, Grenoble, FR
Supervisor: Dr. Jean-Marie Mouesca /jean-marie.mouesca@cea.fr

Title: Study of molecular magnetism by DFT methods, serving as an introduction to the Ph.D thesis

- Calculation of exchange coupling constants by DFT-BS
- Quantitative harmonization of the three molecular orbital, valence bond, and broken symmetry approaches

M. Sc. 1st thesis
May 2007 - July 2007

Organic Electrochemisty Laboratory, Grenoble, FR
Supervisor: Dr. Christine Mousty /Christine.Mousty@univ-bpclermont.fr

Biosensor conception

- Conception of clay-modified electrodes biosensors
- Electrochemistry and Enzymatic activity

TECHNICAL / COMPUTER SKILLS

Computer operating systems: Unix, Mac, Windows

Computer software: MS Office, Open Office, LaTeX, vim, Maxima, vmd, rasmol, pymol

Computer Languages: (I)Python, fortran, awk, HTML, php, mySQL (website designer)

Quantum/classical mechanic codes: ADF, molcas, ORCA, tinker MD

PUBLICATIONS

2012
Magnetic properties of a doped linear polyarylamine bearing a high concentration of coupled spins (S=1). Vincent Maurel, Mohammad Jouni, Piotr Baran, Nicolas Onofrio, Serge Gambarelli, Jean-Marie Mouesca, David Djurado, Lionel Dubois, Jean-François Jaquot, Gérard Desfonds and Irena Kulszewicz-Bajer, *Phys. Chem. Chem. Phys., 2012, 14, 1399-1407*

2011
Analysis of the Singlet-Triplet Splitting Computed by the Density Functional Theory-Broken-Symmetry Method : Is it an Exchange Coupling Constant ? Nicolas Onofrio, Jean-Marie Mouesca, *Inorg. Chem., 2011, 50, 5577-5586*

2010
Valence Bond/Broken Symmetry Analysis of the Exchange Coupling Constant in Copper(II) Dimers. Ferromagnetic Contribution Exalted through Combined Ligand Topology and (Singlet) Covalent-Ionic Mixing. Nicolas Onofrio, Jean-Marie Mouesca, *J. Phys. Chem. A, 2010, 114, 6149-6156*

COMMUNICATIONS

2011
Oral communication
Analysis of the singlet-triplet splitting computed by the DFT - broken symmetry method : Is Jbs an exchange coupling constant ? Nicolas Onofrio, WATOC-2011 Santiago de Compostela, Spain

2011
Poster
Analytical expression of exchange coupling interaction constants in a broken symmetry formalism. Nicolas Onofrio, *Workshop GDR-DFT Lyon, France*

2011
Oral communication
Analysis of te exchange interaction computed by DFT-broken symmetry. Application to copper(II) dimers. Nicolas Onofrio, *GECOM-2011 Merlimont, France*

2011
Poster
Modelization of the exchange interaction by DFT. Nicolas Onofrio, *University Joseph Fourier Grenoble, France*

2010
Oral communication
Analysis of the exchange interaction by density fonctionnal theory (DFT). Nicolas Onofrio, *JFJPC11-2010 Autrans, France*