Curriculum

Vitae

Personal Information

First name(s) / **Adrian**

Surname(s) **CALBOREAN**

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Nationality Romanian

Marital status Married

Date of birth February 14, 1981

Gender Male

Domains of activity

Scientific Title Scientific Researcher, **PhD** at „*Université Joseph Fourier"* and *Commissariat à l'énergie atomique et aux énergies alternatives* Grenoble, France

PostDoc at Ecole Nationale Supérieure de Chimie de Paris (ENSCP), France

Keywords Quantum chemical DFT, TD-DFT, Solid State Physics, Molecular Electronics, Photochemical Molecular Devices, OLEDs, Photovoltaic's

Domains of competence

- Quantum chemistry and solid state DFT and in hybrid molecular electronic capacitive devices.
- Solid State Physics theory for band structure calculations of bulk semiconductor surfaces.

- Structural analysis through TD-DFT - provide a deep insight into the excited state character involved on the absorption and emission processes, dynamics and relaxation pathways.

Domains of Interest

Physicist Engineer with good computational skills and solid scientific background in first-principles simulations. Received a Marie Curie fellowship for my thesis research in modeling semiconducting – nanowires based multilevel molecular memories at the prestigious CEA in France. My research interests lie in the field of computational chemistry (DFT) simulations and solid state physics approach for band structure calculations. In the last years, I was in particular focused on dip pen nanolitography techniques and exprimental characterization of new material alloys by cyclic voltammetry and impedance spectroscopy with direct applications in molecular and bio –electronic fields.

Selected Publications

1. L.Buimaga-Iarinca, N. Ivošević DeNardis, P. T. Vernier, **A. Calborean**, C. Morari, *The Effect of the Electric Field on the α-GPC Interaction with Au(111) Surface: A First-Principles Study,* J. Phys. Chem. C 120 (2016) 9740-9749
2. M. Streza, C. Nut, C.Tudoran, V. Bunea, **A. Calborean**, C. Morari, *Distribution of current in the electrodes of lead-acid batteries: a thermographic analysis approach*, J. Phys. D: Appl. Phys (2016) 49, 055503
3. **A. Calborean**, F. Martin, Marconi D., Turcu R., Kacso I. E., Buimaga-Iarinca L., Graur F., Turcu I., *Adsorption mechanisms of L-Glutathione on Au and controlled nano-patterning through Dip Pen Nanolithography*, Mat. Science& Eng. C-Mat. For Biol.applic. (2015) 57, 171-180
4. C.Morari, C.M.Muntean, C.Tripon, L. Buimaga-Iarinca, **A.Calborean**, *DFT investigation of the vibrational properties of GC Watson-Crick and Hoogsteen base pairs in the presence of Mg2+, Ca2+, and Cu2+ ions*, J. Mol. Model (2014) 20:2220
5. J. Fortage, F. Tuyeras, C. Peltier, G. Dupeyre, **A. Calborean**, F. Bedioui, P. Ochsenbein, F. Puntoriero, S. Campagna, I. Ciofini, P. P. Laine, *Tictoid Expanded Pyridiniums: Assessing Structural, Electrochemical, Electronic, and Photophysical Features*, J. Phys. Chem. A (2012), 116, 7880−7891
6. L. Buimaga-Iarinca, **A. Calborean**, *Electronic structure of the ll-cysteine dimers adsorbed on Au(111): a density functional theory study*, Phys. Scr. (2012) 86, 035707.

7. M. Oltean, **A. Calborean**, G. Mile, M. Vidrighin, M. Iosin, L. Leopold, D. Maniu, N. Leopold, V. Chiş, Absorption spectra of PTCDI: A combined UV–Vis and TD-DFT study, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy (2012), 97, 703 - 710.
8. E. S. Andreiadis, D. Imbert, J. Pécaut, **A. Calborean*,** I. Ciofini, C. Adamo, R. Demadrille, M. Mazzanti, Phosphorescent binuclear iridium complexes based on terpyridine-carboxylate: an experimental and theoretical study, Inorg.Chem. (2011), 50, 17, 8197 - 8206.
9. M. Kepenekian, **A. Calborean**, V. Vetere, B. Le Guennic, V. Robert, P. Maldivi, Ab initio Inspection of Manganese Porphyrin Spin States: Towards Candidates for Redox Bistability, Journal of Chemical Theory and Computation (2011), 7, 11, 3532-3539.
10. T. Pro, J. Buckley, R. Barattin, **A. Calborean**, V. Aiello, G. Nicotra, K. Huang, M. Gély, G.Delapierre, E. Jalaguier, F. Duclairoir, N. Chevalier, S. Lombardo, P. Maldivi, G. Ghibaudo, “From atomistic to device level investigation of hybrid redox molecular/silicon field effect memory device”, IEEE T. on Nanotechnology (2011), 10, 2, 275-283.

Education and Training

PhD DIPLOMA (Chemistry and Natural Sciences Doctoral School, specialty Computational Chemistry) **2009**: Joseph Fourier University of Grenoble and CEA Grenoble, France.

Trainings on: Project Management, Intellectual Property, European Funding

Post-doc ANR (Agence Nationale de la Recherche) Grant -2010: École Nationale Supérieure de Chimie de Paris (ENSCP), France, Laboratoire d’électrochimie, chimie des interfaces et modélisation pour l'énergie” (LECIME).

Activities: Excited states of Ir complexes using TDDFT (OLEDs)
Photochemical Molecular Devices (PMDs)
Photo-magnetic molecular devices (PMMDs)
Photovoltaics through Ru and Ir complexes

Post-doc POSDRU Grant -2011: Babes- Bolyai University, Faculty of Physics, Department of Biomedical Physics, Cluj – Napoca, Romania, 18 months.

Activities: Molecular Electronics
Charge transfer in hybrid structures
Quantum DFT modeling

Researcher – 2011 National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania.

Activities: **Computational chemistry calculations**: *ab-initio* and semiempirical methods, Density Functional Theory, TD-DFT, molecular modeling.

Solid state physics calculations: band structure calculations, intermolecular interactions, molecular dynamics, surface reconstructions, molecular-scale electronics into a functioning structure.

Nov. **2012 – May 2013 - 6 month courses of "Business Management in the domain of durable development"** financed by EU.

Dates / Occupation or position held/ Name of employer	Since 2011, scientific researcher CSIII at National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM), Cluj –Napoca, Romania. 2009-2010 Researcher at École Nationale Supérieure de Chimie de Paris (ENSCP), France. 2006 -2009 Researcher at Commissariat à l'énergie atomique CEA/INAC /SCIB Grenoble, France.

FELLOWSHIPS

2004-2005 European Union Socrates/ Erasmus Scholarship at University of Zaragoza, Spain

2006-2009 Marie Curie fellowship (*Chemtronics* Chemistry and Nanoelectronics European programme) at CEA Grenoble, France

Mother tongue Romanian

Other Language (s)	Self assesment	Understanding	Speaking	Writing
Language	English	Very good	Very good	Very good
Language	French	Very good	Good	Good
Language	Spanish	Very good	Very good	Good

Date 07st February 2017