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Afiliere curentă

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Adresa permanentă: Sat Viișoara, Com. Tg. Trotuș, Jud. Bacău, Romania

Experiența profesională

2017-prezent: Cercetător în regim post doctoral în chimie teoretică și modelare computațională.

Îndrumător: Prof. Jochen Autschbach.

Departamentul de Chimie, State University of New York at Buffalo, Buffalo, Statele Unite ale Americii.

Activități de cercetare în domeniul structurii electronice, legăturilor chimice și proprietăților magnetice ale speciilor chimice ce conțin metale grele.

2013-2016 Cercetător CNRS; chimie teoretică și modelare computațională.

SUBATECH Nantes UMR6457 CNRS IN2P3, Departamentul de Radiochimie, École des Mines de Nantes, Nantes, Franța; CEISAM Nantes, UMR6230 CNRS, Université de Nantes, Franța.

Îndrumători: Dr. Rémi Maurice, Dr. Nicolas Galland

Activitate de cercetare în vederea obținerii titlului de doctor în chimie.

Educație

2013-2016 **Doctorat** în chimie teoretică

Instituția: Université de Nantes, Franța

Teza de doctorat: “Geometries, electronic structures, and physico-chemical properties of astatine species: An application of relativistic quantum mechanics”

Îndrumători: Dr. Nicolas Galland, Dr. Rémi Maurice

Data susținerii tezei de doctorat: 19 Octombrie 2016

2011-2013 **Masterat** în chimie - European Master in Theoretical Chemistry and Computational Modelling (EMTCCM)

Instituția: Facultatea de matematică și științe naturale, University of Groningen, Olanda

Îndrumători ai tezei de masterat: Prof. Ria Broer, Dr. Remco Havenith, Dr. Daniel Roca Sanjuán.

2008-2011 **Licențiat** în chimie

Instituția: Facultatea de Chimie, Universitatea Alexandru Ioan Cuza din Iași, Romania

Îndrumător al tezei de licență: Prof. Ionel Humelnicu

Orientarea activității de cercetare

En. „*My current research concerns the application of ab initio quantum mechanical approaches to get insights on peculiar electronic structures, bonding and magnetic properties, of heavy element systems. In my early years of academic research, I worked on rationalizing the basic chemistry of astatine (At, Z=85), an “invisible” heavy main-group 6p element with promising applications in nuclear medicine. More recently, my research is oriented toward rationalizing the extent of bonding covalency involving actinide 5f vs. transitional metal 3d orbitals. The computational prediction of actinide X-ray absorption spectra, using fully ab initio approaches, lays within my current research projects. My predictive calculations, in the gas phase and in aqueous solution, are based on state-of-the-art relativistic density functional theory and ab initio spin-orbit coupled multiconfigurational wave-function-based approaches.”*

Abilități tehnice

Sisteme de operare:	Linux, Mac OS, Windows
Limbaje de programare:	C++, Python, Fortran, AWK, shell scripting, LaTeX
Softuri chimie computațională:	DIRAC, ADF, Turbomole, Molpro, Molcas, OpenMolcas, Gaussian, NWChem, Orca, GAMESS US, GAMESS UK, MultiWFN, NBO, Exatomic

Limbi cunoscute

Lb. Romană (limbă maternă), Lb. Engleză (vorbit, scris, citit fluent), Lb. Franceză (vorbit, citit fluent)

Participare la scoli de pregătire ştiinţifică

Septembrie 2015	TALISMAN ThUL School in Actinide Chemistry
	Karlsruher Institute Für Technologie, Karlsruhe, Germany
Iulie 2014	SOSTRUP Summer School: Quantum Chemistry and Molecular Properties
	Himmelbjergegnens Natur-og Idrætsefterskole, Denmark
Septembrie 2012	7th International Intensive Course of the TCCM European master
	Department of Chemistry, University of Perugia, Italy
Iunie 2012	European Summer School: TCCM School on Solid State Chemistry
	ZCAM Institute, Zaragoza, Spain
Iunie 2012:	European Summer School: TCCM School on Molecular Excited States
	ZCAM Institute, Zaragoza, Spain.

Stagiu de Cercetare

Ianuarie 2013	Stagiu de cercetare desfăşurat pe o perioada de cinci luni in domeniul fotochimiei.
	Instituția: Instituto de Ciencia Molecular (ICMol), Universitat de València, Spain
	Îndrumători: Prof. Manuela Merchán, Dr. Daniel Roca-Sanjuán

En. „*Using "state-of-the-art" multiconfigurational and multireference wave-function-based methods, I have investigated the efficient phosphorescent-state population in the photoexcited benzophenone molecule. This research has ended up with a manuscript published in Phys. Chem. Chem. Phys. and with an awarded oral communication at the 9th European Conference on Computational Chemistry, Sopron, Hungary, 2−6 September, 2013.*"

Referent Ştiinţific: *Phys. Chem. Chem. Phys., J. Chem. Phys., J. Chem. Theory Comput., Chem. Comm.*

Imagini de tip cover, inside cover

Chem. Eur. J. DOI: 10.1002/chem.201600198

Phys. Chem. Chem. Phys. DOI: 10.1039/c6cp05028j

J. Comput. Chem. DOI: 10.1002/jcc.25103

Publicații (articole in preparare nu sunt menționate)

15. „Use of ^{15}N NMR Spectroscopy to Probe Covalency in a Thorium Nitride", S. Staun, D.-C. Sergentu, G. Wu, J. Autschbach and T. W. Hayton*, Chem. Sci.*, manuscript just accepted.

14. "Homoleptic aryl complexes of uranium(IV)", N. J. Wolford, D.-C. Sergentu, W. Brennessel, J. Autschbach and M. Neidig, *Angew. Chem. Intl. Ed.*, **2019**, DOI: 10.1002/anie.201905423.

13. "Magnetic circular dichroism spectra of transition metal complexes calculated from restricted active space wavefunctions", Y. Heit,* D.-C. Sergentu* and J. Autschbach, *Phys. Chem. Chem. Phys.*, **2019**, 21, 5586. *(*signed as first author)*

12. "*Ab initio* study of covalency in the ground versus core-excited states X-ray absorption spectra of actinide complexes", D.-C. Sergentu, T. J. Duignan and J. Autschbach, *J. Phys. Chem. Lett*., **2018**, 9, 5583.

11. "A diuranium carbide cluster stabilized inside a C_{80} fullerene cage", X. Zhang, W. Li, L. Feng, X. Chen, A. Hansen, S. Grimme, S. Fortier, D.-C. Sergentu, T. J. Duignan, J. Autschbach, S. Wang, Y. Wang, G. Velkos, A. A. Popov, N. Aghdassi, S. Duhm, X. Li, J. Li, L. Echegoyen, W. H. E. Schwarz and N. Chen, *Nat. Commun.,* **2018**, 9, 2753.

10. "Similar ligand-metal bonding for transition metals and actinides? $5f^1$ $U(C_7H_7)^{2-}$ versus $3d^n$ metallocenes", D.-C. Sergentu, F. Gendron and J. Autschbach, *Chem. Sci.,* **2018**, 9, 6292.

9. "Understanding and Controlling the Emission Brightness and Color of Molecular Cerium Luminophores", Y. Quao,* D.-C. Sergentu,* H. Yin, A. V. Zabula, T. Cheisson, A. Mc Skimming, B. C. Manor, P. J. Carroll, J. A. Anna, J. Autschbach and E. J. Schelter, *J. Am. Chem. Soc.,* **2018**, 140, 4588. *(*signed as first author)*

8. "The bonding picture in hypervalent XF_3 (X = Cl, Br, I, At) fluorides revisited with quantum chemical topology", M. Amaouch, D.-C. Sergentu, D. Steinmetz, R. Maurice, N. Galland, R. Maurice and J. Pilmé, *J. Comput. Chem.,* **2017**, 38, 2753.

7. "Targeted radionuclide therapy with astatine-211: Oxidative dehalogenation of astatobenzoate conjugates", D. Teze, D.-C. Sergentu, V. Kalichuk, J, Barbet, D. Deniaud, N. Galland, R. Maurice and G. Montavon, *Scientific Reports,* **2017**, 7, 2579.

6. "The heaviest possible ternary trihalogen species, $AtIBr^-$, evidenced in aqueous solution: An experimental effort driven by computations", N. Guo, D.-C. Sergentu, D. Teze, R. Maurice, J. Champion, N. Galland and G. Montavon, *Angew. Chem*., **2016**, 55, 15369.

5. "Unravelling the hydration-induced ground-state change of AtO^+ by relativistic and multiconfigurational wave-function-based methods", D.-C. Sergentu, F. Réal, G. Montavon, N. Galland and R. Maurice, *Phys. Chem. Chem. Phys.*, **2016**, 18, 32703.

4. “Scrutinizing “invisible” astatine: A challenge for modern density functionals”, D.-C. Sergentu, G. David, G. Montavon, R. Maurice and N. Galland, *J. Comput. Chem.*, **2016**, 37, 1345.

3. “Advances on the determination of the astatine Pourbaix diagram: Predomination of $AtO(OH)_2^-$ over At^- in basic conditions”, D.-C. Sergentu, D. Teze, A. Sabatié-Gogova, C. Alliot, N. Guo, F. Basal, I. Da Silva, D. Deniaud, R. Maurice, J. Champion, N. Galland and G. Montavon, *Chem. Eur. J.*, **2016**, 22, 2964.

2. “Electronic structures and geometries of the XF_3 (X = Cl, Br, I, At) fluorides”, D.-C. Sergentu, M. Amaouch, J. Pilmé, N. Galland and R. Maurice, *J. Chem. Phys.*, **2015**, 143, 114306.

1. “Computational determination of the dominant triplet population mechanism in photoexcited benzophenone”, D.-C. Sergentu, R. Maurice, R. W. A. Havenith, R. Broer and D. Roca-Sanjuán, *Phys. Chem. Chem. Phys.*, **2014**, 16, 25393.

Contribuții Orale, Conferințe Internaționale

2. “Electronic structures of the XF_3 (X = Cl, Br, I, At) fluorides and topology of their potential energy surfaces", D.-C. Sergentu, N. Galland and R. Maurice, 2nd European Symposium on Density Functional Theory and its Applications, Debrecen, Hungary, 31 August − 4 September, 2015.

1. “Revisiting the intersystem crossing in benzophenone”, D.-C. Sergentu, D. Roca-Sanjuán, R. W. A. Havenith and R. Braam-Broer, 9th European Conference on Computational Chemistry, Sopron, Hungary, 2−6 September, 2013.

Contribuții cu Poster, Conferințe si Workshopuri Internaționale

4. “X-ray absorption spectroscopy: Chemical bonding in actinide complexes from *ab initio* multireference wavefunction approaches”, D.-C. Sergentu and J. Autschbach, 2nd European Symposium on Chemical Bonding, Oviedo, Spain, 3 September − 7 September, 2018.

3. “The peculiar electronic structure of AtO^+ in water”, D.-C. Sergentu, F. Réal, N. Galland and R. Maurice, 7th International Meeting on Atomic and Molecular Physics and Chemistry, Le Havre, France, 27−30 June, 2016.

2. “Ground-state reversal induced by solvation: Electronic structure of AtO^+ in water”, D.-C. Sergentu, N. Galland and R. Maurice, TALISMAN ThUL School in Actinide Chemistry, Karlsruhe, Germany, 28 September − 2 October, 2015.

1. “Investigation of the $AtO(OH)_2^-$ hydrolysed species: Relativistic calculations”, D.-C. Sergentu, J. Champion, A. Sabatié-Gogova, J.-Y. Le Questel, R. Maurice, G. Montavon and N. Galland, SOSTRUP Summer School: Quantum Chemistry and Molecular Properties, Himmelbjergegnens Natur-og Idrætsefterskole, Denmark, 6−18 July, 2014.

Alte seminarii susţinute in fata unui public larg

4. “Investigating AtO^+-$(OH^-)_n$ complexes at the molecular scale using quantum mechanical methods”, D.-C. Sergentu, J. Champion, A. Sabatié-Gogova, J.-Y. Le Questel, R. Maurice, G. Montavon and N. Galland, Scientific days of The 3MPL doctorate school, Le Mans, France, June 2015. Oral communication in front of PhD students of the 3MPL doctorate school from Nantes, Le Mans and Anger.

3. “Theoretical investigation of the AtO^+ hydrolysed species in ligand-exchange reactions including solvation effects”, D.-C. Sergentu, J. Champion, A. Sabatié-Gogova, J.-Y. Le Questel, R. Maurice, G. Montavon and N. Galland, Scientific Days of The 3MPL Doctorate School, Nantes, France, June 2014. Poster presentation in front of PhD students of the 3MPL doctorate school from Nantes, Le Mans and Anger.

2. “*Pseudo* Jahn-Teller effect, spin-orbit coupling and electron correlation in the XF_3 (X = Cl, Br, I, At) series”, D.-C. Sergentu, R. Maurice and N. Galand, University of Groningen, The Netherlands, April 2014. Seminar given in front of the research group of Prof. Ria Braam-Broer.

1. “Revisiting the intersystem crossing in benzophenone", D.-C. Sergentu, R. Maurice, R. W. A. Havenith, R. Broer and D. Roca-Sanjuán, IFW Dresden, Germany, March 2013. Invited seminar given in front of scientists from the Leibniz Institute for solid state and material research, Dresden, Germany.

Persoane de Contact

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2. Dr. Nicolas Galland, CEISAM, UMR CNRS 6230, Université de Nantes − Faculté des Sciences et des Techniques, 2 rue de la Houssiniére, BP 92208, 44322 Nantes Cedex 3, France, E-mail: nicolas.galland@univ-nantes.fr.

3. Dr. Rémi Maurice, SUBATECH, UMR CNRS 6457, IN2P3/Mines Nantes/Université de Nantes, 4 rue Alfred Kastler, BP 20722, 44307 Nantes Cedex 3, France, E-mail: remi.maurice@subatech.in2p3.fr.

4. Prof. Ria Braam-Broer, Department of Theoretical Chemistry, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands, E-mail: r.broer@rug.nl.