

Nume Prenume: Sergentu Dumitru-Claudiu

Gradul didactic: Lector universitar doctor

Instituția unde este titular: Universitatea „Alexandru Ioan Cuza” din Iași

Facultatea: Chimie

Departamentul: Chimie

L I S T A LUCRĂRILOR ȘTIINȚIFICE

A. Teza de doctorat

Titlu: „Geometries, electronic structures and physico-chemical properties of astatine species: An application of relativistic quantum mechanics”

Instituția: Universitatea din Nantes, Franța

Data susținerii: 19 octombrie 2016

Școala doctorală: Matériaux, Matières, Molécules en Pays de la Loire (3MPL)

Link URL: <https://theses.fr/2016NANT4024>

B. Cărți și capitole în cărți publicate în ultimii 5 ani (2021-2025)

C. Lucrări indexate ISI/BDI publicate în ultimii 5 ani (2021-2025)

1. P. W. Smith, D.-C. Sergentu, J. A. Branson, D. R. Russo, C. H. Booth, J. Autschbach and S. G. Minasian „4f-Orbital Occupancy in Tetravalent Cerium Halide Complexes from X-ray Spectroscopy and Theory”, *Inorg. Chem.* 2025, **64**, 18091.
2. H. Gupta, A. Sen, P. W. Smith, B. D. Vincenzini, N. Mavragani, D.-C. Sergentu, A. M. Bacon, C. H. Booth, M. Murugesu, S. G. Minasian, J. Autschbach and E. J. Schelter „An Ytterbium-Pyrazine Square $[(C_5H_4Me)_2Yb^{III}(pyz^-)]_4$ Formed by Reversible Electron Transfer and Concomitant Self-Assembly”, *Inorg. Chem.* 2025, **64**, 14753.
3. M. Paiu, L. Favier, D. Lutic, R. M. Hlihor, D.-C. Sergentu, V. Alonzo and M. Gavrilescu „First insight on the effective removal of pentoxifylline drug under visible-light-driven irradiation with ZnO catalyst obtained via precipitation”, *J. Environ. Manag.* 2025, **386**, 125420.
4. A. M. Toader, M. C. Buta, I. Humelnicu, W. Urland, M. Suta, D.-C. Sergentu (*co-corespondent) and F. Cimpoesu „Ab Initio Modeling of the Photoluminescence of $SrCl_2:Eu^{2+}$ -Direct Comparison between Density Functional and Wave Function Theory-Based Approaches”, *Inorg. Chem.* 2025, **64**, 5996.
5. D. R. Russo, A. N. Gaiser, A. N. Price, D.-C. Sergentu (*autor prim cu contribuții egale), J. N. Wacker, N. Katzer, A. A. Peterson, J. A. Branson, X. Yu, S. N. Kelly, E. T. Ouellette, J. Arnold, J. R.

- Long, W. W. Lukens, S. J. Teat, R. J. Abergel, P. L. Arnold, J. Autschbach and S. G. Minasian „Berkelium–carbon bonding in a tetravalent berkelocene”, *Science* 2025, **387**, 974.
6. J. A. Bronson, P. W. Smith, D.-C. Sergentu, D. R. Russo, Himanshu Gupta, Corwin H. Booth, J. Arnold, E. J. Schelter, J. Autschbach and S. G. Minasian „The counterintuitive relationship between orbital energy, orbital overlap, and bond covalency in CeF_6^{2-} and CeCl_6^{2-} ”, *J. Am. Chem. Soc.* 2024, **146**, 25640.
7. D.-C. Sergentu, B. Le Guennic and R. Maurice „The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes”, *Phys. Chem Chem. Phys.*, 2024, **26**, 6844.
8. G. Li Manni, I. F. Galván, ..., D.-C. Sergentu, ..., and R. Lindh „The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry”, *J. Chem. Theory Comput.*, 2023, **19**, 6933.
9. A. Ramanathan, J. Kaplan, D.-C. Sergentu, J. A. Branson, M. Ozerov, A. I. Kolesnikov, S. G. Minasian, J. Autschbach, J. W. Freeland, Z. Jiang, M. Mourigal and H. S. La Pierre „Chemical design of electronic and magnetic energy scales in tetravalent praseodymium”, *Nature Commun.*, 2023, **14**, 3134.
10. Q. Meng, L. Abella, Y.-R. Yao, D.-C. Sergentu, W. Yang, X. Liu, J. Zhuang, L. Echegoyen, J. Autschbach and N. Chen „A charged diatomic triple-bonded $\text{U}\equiv\text{N}$ species trapped in C_{82} fullerene cages”, *Nature Commun.*, 2022, **13**, 7192.
11. D.-C. Sergentu and J. Autschbach „Covalency in actinide(IV) hexachlorides in relation to chlorine K-edge X-ray absorption structure”, *Chem. Sci.* 2022, **13**, 3194.
12. D.-C. Sergentu and J. Autschbach “X-ray absorption spectra of f-element complexes: Insight from relativistic multiconfigurational wavefunction theory”, *Dalton Trans.*, 2022, **51**, 1754.
13. D.-C. Sergentu, F. Gendron, E. D. Walter, S. Park, C. Capan, R. G. Surbella, C. Z. Soderquist, G. B. Hall, S. I. Sinkov, J. Autschbach, and H. Cho „Equatorial electronic structure in the uranyl ion: $\text{Cs}_2\text{UO}_2\text{Cl}_4$ and $\text{Cs}_2\text{UO}_2\text{Br}_4$ ”, *Inorg. Chem.* 2022, **61**, 3821.
14. X. Yu, D.-C. Sergentu, R. Feng, and J. Autschbach „Covalency of trivalent actinide ions with different donor ligands: Do density functional and multiconfigurational wavefunction calculations corroborate the observed “breaks”?”, *Inorg. Chem.*, 2021, **60**, 17744.
15. D.-C. Sergentu (*co-correspondent), C. Booth and J. Autschbach „Probing multiconfigurational states by spectroscopy: The cerium XAS L3-edge puzzle”, *Chem. Eur. J.*, 2021, **27**, 7239.
16. Y. Qiao, G. Ganguly, C. H. Booth, J. A. Branson, A. S. Ditter, D. J. Lussier, L. M. Moreau, D. R. Russo, D.-C. Sergentu, D. K. Shuh, T. Sun, J. Autschbach and S. G. Minasian “Enhanced 5f- δ bonding in $[\text{U}(\text{C}_7\text{H}_7)_2]^-$: C K-edge XAS, magnetism, and ab initio calculations”, *Chem. Commun.*, 2021, **57**, 9562.

17. G. B. Panetti, D.-C. Sergentu, M. R. Gau, J. Autschbach, P. J. Walsh, and E. J. Schelter “Isolation and characterization of a covalent Ce^{IV}-aryl complex with an anomalous ¹³C chemical shift”, *Nat. Commun.* 2021, **12**, 1713.

D. Lucrări publicate în ultimii 5 ani (2021-2025) în reviste și volume de conferințe cu referenți (neindexate)

- Reviste

- Selecție cu maximum 20 lucrări în volume de conferințe

E. Brevete obținute în întreaga activitate

Data: 20.02.2026