Dr. Dumitru-Claudiu Sergentu

LISTA COMPLETĂ DE LUCRĂRI

structurată conform Art. 11 din Metodologia de concurs pentru ocuparea posturilor didactice şi de cercetare în Universitatea ”Alexandru Ioan Cuza” din Iaşi

Lista celor maximum 10 lucrări relevante

1. D.-C. Sergentu and J. Autschbach, “X-ray absorption spectra of f-element complexes: Insight from relativistic multiconfigurational wavefunction theory”, ***Dalton Trans.*** **(IF=4.390)**, 2022, 51, 1754.
2. D.-C. Sergentu and J. Autschbach, “Covalency in actinide(IV) hexachlorides in relation to chlorine K-edge X-ray absorption structure”, ***Chem. Sci.*** **(IF=9.825)**, 2022, 13, 3194.
3. 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: $Cs_2UO_2Cl_4$ and $Cs_2UO_2Br_4$”, ***Inorg. Chem.*** **(IF=5.165)**, 2022, 61, 3821.
4. 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 ^{13}C chemical shift”, ***Nat. Commun.*** **(IF=14.919)**, 2021, 12, 1713.
5. D.-C. Sergentu,* C. Booth and J. Autschbach,* “Probing multiconfigurational states by spectroscopy: The cerium XAS L_3-edge puzzle”, ***Chem. Eur. J.*** **(IF=5.236)**, 2021, 27, 7239. (*autor corespondent)
6. J. M. Sperling, E. J. Warzecha, C. Celis-Barros, D.-C. Sergentu, X. Wang, B. E. Klamm, C. J. Windorff, A. N. Gaiser, F. D. White, D. A. Beery, A. T. Chemey, M. A. Whitefoot, B. N. Long, K. Hanson, P. Kögerler, M. Speldrich, E. Zurek, J. Autschbach and T. E. Albrecht-Schmitt, “Compression of curium pyrrolidinedithiocarbamate enhances covalency”, ***Nature*** **(IF=49.962)**, 2020, 583, 396.
7. D.-C. Sergentu, F. Gendron and J. Autschbach, “Similar ligand-metal bonding for transition metals and actinides? $5f^1$ $U(C_7H_7)^{2-}$ versus $3d^n$ metallocenes”, ***Chem. Sci.*** **(IF=9.825)**, 2018, 9, 6292.
8. 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, “Understanding and Controlling the Emission Brightness and Color of Molecular Cerium Luminophores”, ***J. Am. Chem. Soc.*** **(IF=15.419)**, 2018, 140, 4588. (*contribuție egală)
9. D.-C. Sergentu, T. J. Duignan and J. Autschbach, “*Ab initio* study of covalency in the ground versus core-excited states X-ray absorption spectra of actinide complexes”, ***J. Phys. Chem. Lett*****. (IF=6.475)**, 2018, 9, 5583.
10. N. Guo, D.-C. Sergentu, D. Teze, R. Maurice, J. Champion, N. Galland and G. Montavon, “The heaviest possible ternary trihalogen species, $AtIBr^-$, evidenced in aqueous solution: An experimental effort driven by computations”, ***Angew. Chem. Int. Ed.*** **(IF=15.336)**, 2016, 55, 15369.

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Teza sau tezele de doctorat:
„Geometries, electronic structures and physico-chemical properties of astatine species: An application of relativistic quantum mechanics”, Școala doctorală 3MPL, Universitatea din Nantes, Franța, susţinută public în data de 19 octombrie 2016. Link URL: https://www.theses.fr/2016NANT4024

Articole/studii publicate *in extenso*, în reviste din circuitul internațional:

1. D.-C. Sergentu and J. Autschbach, “Covalency in actinide(IV) hexachlorides in relation to chlorine K-edge X-ray absorption structure”, *Chem. Sci.* **(IF=9.825)**, 2022, 13, 3194.
2. D.-C. Sergentu and J. Autschbach, “X-ray absorption spectra of f-element complexes: Insight from relativistic multiconfigurational wavefunction theory”, *Dalton Trans.* **(IF=4.390)**, 2022, 51, 1754.
3. 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: $Cs_2UO_2Cl_4$ and $Cs_2UO_2Br_4$”, *Inorg. Chem.* **(IF=5.165)**, 2022, 61, 3821.
4. 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.* **(IF=5.165)**, 2021, 60, 17744.
5. D.-C. Sergentu,* C. Booth and J. Autschbach,* “Probing multiconfigurational states by spectroscopy: The cerium XAS L3-edge puzzle”, ***Chem. Eur. J.*** **(IF=5.236)**, 2021, 27, 7239. (*autor corespondent)
6. 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 $[U(C_7H_7)_2]^-$: C K-edge XAS, magnetism, and ab initio calculations”, *Chem. Commun.* **(IF=6.222)**, 2021, 57, 9562.
7. 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 ^{13}C chemical shift”, *Nat. Commun.* **(IF=14.919)**, 2021, 12, 1713.
8. D.-C. Sergentu, G. Kent, S. Staun, X. Yu, H. Cho, J. Autschbach and T. Hayton, “Probing the electronic structure of a thorium nitride complex by solid-state ^{15}N NMR spectroscopy”, *Inorg. Chem.* **(IF=5.165)**, 2020, 59, 10138.
9. C. G. Pech, Pi A. B. Haase, D.-C. Sergentu, A. Borschevsky, J. Pilmé, N. Galland and R. Maurice, “Quantum chemical topology at the spin-orbit configuration interaction level: Application to astatine compounds”, *J. Comput. Chem.* **(IF=3.376)**, 2020, 41, 2055.
10. J. M. Sperling, E. J. Warzecha, C. Celis-Barros, D.-C. Sergentu, X. Wang, B. E. Klamm, C. J. Windorff, A. N. Gaiser, F. D. White, D. A. Beery, A. T. Chemey, M. A. Whitefoot, B. N. Long, K. Hanson, P. Kögerler, M. Speldrich, E. Zurek, J. Autschbach and T. E. Albrecht-Schmitt, “Compression of curium pyrrolidinedithiocarbamate enhances covalency”, *Nature* **(IF=49.962)**, 2020, 583, 396.
11. F. Aquilante, J. Autschbach, A. Baiardi, S. Battaglia, V. Borin, L. Chibotaru, I. Conti, L. De Vico, M. Delcey, I. Fdez. Galván, N. Ferré, L. Freitag, M. Garavelli, X. Gong, S. Knecht, E. Larsson, R. Lindh, M. Lundberg, P.-A. Malmqvist, A. Nenov, J. Norell, M. Odelius, M. Olivucci, T. Pedersen, L. Pedraza-González, Q. Phung, K. Pierloot, M. Reiher, I. Schapiro, J. Segarra-Martí, F. Segatta, L. Seijo, S. Sen, D.-C. Sergentu, C. Stein, L. Ungur, M. Vacher, A. Valentini and V. Veryazov, “Modern quantum chemistry with [Open]Molcas”, *J. Chem. Phys.* **(IF=3.488)**, 2020, 152, 214117.
12. J. Sears, D.-C. Sergentu T. Baker, W. Brennessel J. Autschbach and M. Neidig, “The exceptional diversity of homoleptic uranium-methyl complexes”, *Angew. Chem. Int. Ed.* **(IF=15.336)**, 2020, 59, 13586.

13. G. Ganguly,* D.-C. Sergentu,* and J. Autschbach, "Ab initio analysis of metal-ligand bonding in $An(COT)_2$ with An = Th, U in their ground and core-excited states", *Chem. Eur. J.* **(IF=5.236)**, 2020, 26, 1776. (*contribuție egală)
14. J. Zhuang,* L. Abella,* D.-C. Sergentu,* Y.-R. Yao, M. Jin, W. Yang, X. Zhang, X. Li, D. Zhang, Y. Zhao, Xi. Li, S. Wang, L. Echegoyen, J. Autschbach and N. Chen, "Diuranium(IV) carbide cluster U_2C_2 stabilized inside fullerene cages", *J. Am. Chem. Soc.* **(IF=15.419)**, 2019, 141, 20249. (*contribuție egală)
15. M. K. Assefa, D.-C. Sergentu, L. A. Seaman, G. Wu, J. Autschbach and T. W. Hayton, "Synthesis, characterization, and electrochemistry of the homoleptic f element ketimide complexes $[Li]_2[M(N=C^tBuPh)_6]$ (M = Ce, Th)", *Inorg. Chem.* **(IF=5.165)**, 2019, 58, 12654.
16. S. Staun, D.-C.Sergentu, G. Wu, J. Autschbach and T. W. Hayton, "Use of ^{15}N NMR spectroscopy to probe covalency in a thorium nitride", *Chem. Sci.* **(IF=9.825)**, 2019, 10, 6431.
17. N. J. Wolford, D.-C. Sergentu, W. Brennessel, J. Autschbach and M. Neidig, "Homoleptic aryl complexes of uranium(IV)", *Angew. Chem. Int. Ed.* **(IF=15.336)**, 2019, 58, 10266.
18. Y. Heit,* D.-C. Sergentu* and J. Autschbach, "Magnetic circular dichroism spectra of transition metal complexes calculated from restricted active space wavefunctions", *Phys. Chem. Chem. Phys.* **(IF=3.676)**, 2019, 21, 5586. (*contribuție egală)
19. D.-C. Sergentu, T. J. Duignan and J. Autschbach, "*Ab initio* study of covalency in the ground versus core-excited states X-ray absorption spectra of actinide complexes", *J. Phys. Chem. Lett*. **(IF=6.475)**, 2018, 9, 5583.
20. 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, "A diuranium carbide cluster stabilized inside a C_{80} fullerene cage", *Nat. Commun.* **(IF=14.919)**, 2018, 9, 2753.
21. D.-C. Sergentu, F. Gendron and J. Autschbach, "Similar ligand-metal bonding for transition metals and actinides? $5f^1$ $U(C_7H_7)^{2-}$ versus $3d^n$ metallocenes", *Chem. Sci.* **(IF=9.825)**, 2018, 9, 6292.
22. 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, "Understanding and Controlling the Emission Brightness and Color of Molecular Cerium Luminophores", *J. Am. Chem. Soc.* **(IF=15.419)**, 2018, 140, 4588. (*contribuție egală)
23. M. Amaouch, D.-C. Sergentu, D. Steinmetz, R. Maurice, N. Galland, R. Maurice and J. Pilmé, "The bonding picture in hypervalent XF_3 (X = Cl, Br, I, At) fluorides revisited with quantum chemical topology", *J. Comput. Chem.* **(IF=3.376)**, 2017, 38, 2753.
24. D. Teze, D.-C. Sergentu, V. Kalichuk, J, Barbet, D. Deniaud, N. Galland, R. Maurice and G. Montavon, "Targeted radionuclide therapy with astatine-211: Oxidative dehalogenation of astatobenzoate conjugates", ***Sci. Rep.*** **(IF=4.380)**, 2017, 7, 2579.
25. N. Guo, D.-C. Sergentu, D. Teze, R. Maurice, J. Champion, N. Galland and G. Montavon, "The heaviest possible ternary trihalogen species, $AtIBr^-$, evidenced in aqueous solution: An experimental effort driven by computations", *Angew. Chem. Int. Ed.* **(IF=15.336)**, 2016, 55, 15369.
26. D.-C. Sergentu, F. Réal, G. Montavon, N. Galland and R. Maurice, "Unravelling the hydration-induced ground-state change of AtO^+ by relativistic and multiconfigurational wave-function-based methods", *Phys. Chem. Chem. Phys*. **(IF=3.676)**, 2016, 18, 32703.
27. D.-C. Sergentu, G. David, G. Montavon, R. Maurice and N. Galland, "Scrutinizing "invisible" astatine: A challenge for modern density functionals", *J. Comput. Chem*. **(IF=3.376)**, 2016, 37, 1345.
28. 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, "Advances on the determination of the astatine Pourbaix diagram: Predomination of $[AtO(OH)_2]^-$ over At^- in basic conditions", *Chem. Eur. J.* **(IF=5.236)**, 2016, 22, 2964.

29. D.-C. Sergentu, M. Amaouch, J. Pilmé, N. Galland and R. Maurice, "Electronic structures and geometries of the XF_3 (X = Cl, Br, I, At) fluorides", *J. Chem. Phys.* **(IF=3.488)**, 2015, 143, 114306.
30. D.-C. Sergentu, R. Maurice, R. W. A. Havenith, R. Broer and D. Roca-Sanjuán, "Computational determination of the dominant triplet population mechanism in photoexcited benzophenone", *Phys. Chem. Chem. Phys.* **(IF=3.676)**, 2014, 16, 25393.

Alte lucrări şi contribuţii ştiinţifice
Participări la manifestări ştiinţifice internaţionale

1. Poster: "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.
2. Poster: "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.
3. Poster plus Workshop: "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.
4. Comunicare orală: "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.
5. Comunicare orală: "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.
6. Poster plus Workshop: "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.
7. Poster: "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.
8. Comunicare orală: "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.
9. Workshop: "TCCM School on Molecular Excited States" held in ZCAM, Zaragoza, Spain, co-organized by the Erasmus Mundus Master in Theoretical Chemistry and Computational Modeling (TCCM), June 2012.
10. Workshop: "TCCM School on Solid State Chemistry" held in ZCAM, Zaragoza, Spain, co-organized by the Erasmus Mundus Master in Theoretical Chemistry and Computational Modeling (TCCM), June 2012.

Data, **Dr. Dumitru-Claudiu Sergentu**
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