FIŞĂ DE AUTOEVALUARE

privind standardele minimale pe domenii ale Universităţii, pentru funcţiile de cercetare

ANEXA 2

Facultatea de Chimie **ASISTENT DE CERCETARE**	
Standarde minimale:	2 articole ştiinţifice publicate în *extenso* în reviste internaţionale, din care 1 în reviste cotate *Web of Science* cu factor de impact
Rezultat autoevaluare:	30 articole ştiinţifice publicate în *extenso* în reviste internaţionale, toate sunt cotate ISI, 16 ca autor principal, factor de impact cumulat: 272.09

Articole ştiinţifice publicate în extenso în reviste internaţionale, cotate *Web of Science* cu factor de impact (factorii de impact (IF) sunt cei curenți și au fost preluați de pe pagina web oficială a fiecărei edituri în parte):

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.
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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.

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