

Fișa de autoevaluare privind standarde minimale pe domenii ale Universității

Posturi didactice pe durată nedeterminată

ANEXA 1A

Facultatea de Chimie ASISTENT UNIVERSITAR	
Standarde minimale:	1. minim 3 articole științifice publicate în <i>extenso</i> în reviste internaționale, cu factor ISI cumulată minim 4; 2. autor principal la 2 articole științifice publicate în <i>extenso</i> în reviste internaționale cotate ISI.
Rezultat autoevaluare:	1. 31 articole științifice publicate în <i>extenso</i> în reviste internaționale, toate sunt cotate ISI. ISI cumulată: 326.5 2. autor principal la 16 articole, toate sunt publicate în reviste internaționale cotate ISI.

Articole științifice publicate în *extenso* în reviste internaționale, 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):

- 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 U≡N species trapped in C82 fullerene cages", *Nature Commun.* (IF=17.694), 2022, 13, 7192.
- [D.-C. Sergentu](#) and J. Autschbach, "Covalency in actinide(IV) hexachlorides in relation to chlorine K-edge X-ray absorption structure", *Chem. Sci.* (IF=9.969), 2022, 13, 3194.
- [D.-C. Sergentu](#) and J. Autschbach, "X-ray absorption spectra of f-element complexes: Insight from relativistic multiconfigurational wavefunction theory", *Dalton Trans.* (IF=4.569), 2022, 51, 1754.
- [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: Cs₂UO₂Cl₄ and Cs₂UO₂Br₄", *Inorg. Chem.* (IF=5.436), 2022, 61, 3821.
- 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=5.436), 2021, 60, 17744.
- [D.-C. Sergentu](#),* C. Booth and J. Autschbach,* "Probing multiconfigurational states by spectroscopy: The cerium XAS L3-edge puzzle", *Chem. Eur. J.* (IF=5.02), 2021, 27, 7239. (*autor corespondent)
- 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(C₇H₇)₂]⁺: C K-edge XAS, magnetism, and ab initio calculations", *Chem. Commun.* (IF=6.065), 2021, 57, 9562.
- 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.* (IF=17.694), 2021, 12, 1713.
- [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 ¹⁵N NMR spectroscopy", *Inorg. Chem.* (IF=5.436), 2020, 59, 10138.
- 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=3.672), 2020, 41, 2055.
- J. M. Sperling, E. J. Warzecha, C. Celis-Barros, [D.-C. Sergentu](#), X. Wang, B. E. Klammer, 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=69.504), 2020, 583, 396.
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- 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=4.304), 2020, 152, 214117.
13. 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=16.823), 2020, 59, 13586.
 14. 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=5.02), 2020, 26, 1776. (*contribuție egală)
 15. 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=16.383), 2019, 141, 20249. (*contribuție egală)
 16. 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=5.436), 2019, 58, 12654.
 17. 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=9.969), 2019, 10, 6431.
 18. N. J. Wolford, [D.-C. Sergentu](#), W. Brennessel, J. Autschbach and M. Neidig, "Homoleptic aryl complexes of uranium(IV)", *Angew. Chem. Int. Ed.* (IF=16.823), 2019, 58, 10266.
 19. 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=3.945), 2019, 21, 5586. (*contribuție egală)
 20. [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=6.888), 2018, 9, 5583.
 21. 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=17.694), 2018, 9, 2753.
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 23. 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=16.383), 2018, 140, 4588. (*contribuție egală)
 24. 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=3.672), 2017, 38, 2753.
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 31. [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=3.945), 2014, 16, 25393.