ANEXA 2 STANDARDE MINIMALE

DR. SERGENTU DUMITRU-CLAUDIU

FACULTATEA	FUNCTIA DE CERCETARE	STANDARDE MINIMALE
CHIMIE	ASISTENT	1. Minim trei articole publicate in extenso în reviste internațional, cu factor ISI cumulat minim 4; 2. Autor principal la doua articole științifice publicate in extenso în reviste internațional cotate ISI

Articole publicate in extenso in reviste cu factor ISI

TOTAL ISI CUMULAT 98.971

1. “Homoleptic aryl complexes of uranium(IV)”, N. J. Wolford, D.-C. Sergentu, W. Brennessel, J. Autschbach and M. Neidig, ***Angew. Chem. (IF=12.102)***, 2019, DOI: 10.1002/anie.201905423.
2. “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. (IF=3.906)***, 2019, 21, 5586. *(*semnat ca prim autor)*

3. “*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. (IF=8.709)***, 2018, 9, 5583.

4. “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. (IF=12.353),*** 2018, 9, 2753.

5. “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. (IF=9.063)***, 2018, 9, 6292.

6. "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. (IF=14.357),*** 2018, 140, 4588. *(*semnat ca prim autor)*

7. "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. (IF=3.221),*** 2017, 38, 2753.

8. "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, ***Sci. Rep. (IF=4.122),*** 2017, 7, 2579.

9. "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. (IF=12.102)***, 2016, 55, 15369.

10. "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. (IF=3.906)***, 2016, 18, 32703.

11. "Scrutinizing "invisible" astatine: A challenge for modern density functionals", D.-C. Sergentu, G. David, G. Montavon, R. Maurice and N. Galland, ***J. Comput. Chem. (IF=3.221)***, 2016, 37, 1345.

12. "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. (IF=5.160)***, 2016, 22, 2964.

13. "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. (IF=2.843)***, 2015, 143, 114306.

14. "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. (IF=3.906)***, 2014, 16, 25393.

Autor principal la doua articole stiintifice publicate in extenso in reviste internationale cotate ISI
TOTAL ISI CUMULAT 55.071

1. "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. (IF=3.906)***, 2019, 21, 5586. *(*semnat ca prim autor)*

2. "*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. (IF=8.709)***, 2018, 9, 5583.

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4. "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. (IF=14.357)***, 2018, 140, 4588. *(*semnat ca prim autor)*

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. (IF=3.906)***, 2016, 18, 32703.

6. "Scrutinizing "invisible" astatine: A challenge for modern density functionals", D.-C. Sergentu, G. David, G. Montavon, R. Maurice and N. Galland, ***J. Comput. Chem. (IF=3.221)***, 2016, 37, 1345.

7. "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. (IF=5.160)***, 2016, 22, 2964.

8. "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. (IF=2.843)***, 2015, 143, 114306.

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