

## LISTA ARTICOLE PUBLICATE IN JURNALE COTATE ISI

DR. SERGENTU DUMITRU-CLAUDIU

15. „Use of  $^{15}\text{N}$  NMR Spectroscopy to Probe Covalency in a Thorium Nitride”, S. Staun, D.-C. Sergentu, G. Wu, J. Autschbach and T. W. Hayton, *Chem. Sci.* (IF=9.063), manuscript just accepted.
14. “Homoleptic aryl complexes of uranium(IV)”, N. J. Welford, D.-C. Sergentu, W. Brennessel, J. Autschbach and M. Neidig, *Angew. Chem.* (IF=12.102), 2019, DOI: 10.1002/anie.201905423.
13. “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. (\*signed as first author)
12. “*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.
11. “A diuranium carbide cluster stabilized inside a  $\text{C}_{80}$  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.
10. “Similar ligand-metal bonding for transition metals and actinides?  $5f^1 \text{U}(\text{C}_7\text{H}_7)^{2-}$  versus  $3d^n$  metallocenes”, D.-C. Sergentu, F. Gendron and J. Autschbach, *Chem. Sci.* (IF=9.063), 2018, 9, 6292.
9. “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. (\*signed as first author)
8. “The bonding picture in hypervalent  $\text{XF}_3$  (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.
7. “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.
6. “The heaviest possible ternary trihalogen species,  $\text{AtI}^-\text{Br}^-$ , 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.
5. “Unravelling the hydration-induced ground-state change of  $\text{AtO}^+$  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.

4. "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.
3. "Advances on the determination of the astatine Pourbaix diagram: Predomination of  $\text{AtO}(\text{OH})_2^-$  over  $\text{At}^-$  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.
2. "Electronic structures and geometries of the  $\text{XF}_3$  ( $\text{X} = \text{Cl}, \text{Br}, \text{I}, \text{At}$ ) fluorides", D.-C. Sergentu, M. Amaouch, J. Pilmé, N. Galland and R. Maurice, ***J. Chem. Phys.*** (***IF=2.843***), 2015, 143, 114306.
1. "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.