FIŞĂ DE AUTOEVALUARE

în conformitate cu prevederile fişei de evaluare generală a standardelor Universităţii

ANEXA 1

DESCRIPTORI		PUNCTAJ
1.	Articole ştiinţifice publicate *in extenso* în reviste cotate *Web of Science* cu factor de impact	2786.87
2.	Articole ştiinţifice publicate *in extenso* în reviste indexate fără factor de impact	0
3.	Articole ştiinţifice publicate *in extenso* în reviste indexate BDI	0
4.	Articole ştiinţifice publicate *in extenso* în volumele conferinţelor	0
5.	Cărţi ştiinţifice publicate (doar prima ediţie)	0
6.	Cărţi ştiinţifice traduse şi publicate în edituri din străinătate	0
7.	Coordonarea şi editarea de volume, traduceri şi antologii	0
8.	Articole publicate în dicţionare şi enciclopedii	0
9.	Contracte de cercetare ştiinţifică în instituţii academice (universităţi, institute ale Academiei Române, institute naţionale de cercetare, institute de cercetare din străinătate, alte categorii de institute academice)	0
10.	Contracte de cercetare în mediul de afaceri şi sectorul public	0
11.	Brevete	0
12.	Citări şi recenzii ale lucrărilor ştiinţifice	9496.08
13.	Lucrări susţinute în calitate de invitat la manifestări ştiinţifice (conferinţe, congrese, simpozioane, seminarii şi ateliere de lucru)	0
14.	Profesor/cercetător invitat la universităţi/institute de cercetare	0
15.	Editor/Membru în *Editorial Board & Advisory Board*	0
16.	Premii internaţionale obţinute printr-un proces de selecţie	0
17.	Premii ale Academiei Române	0
18.	Alte premii naţionale ale instituţiilor culturale	0
19.	Participări la manifestări ştiinţifice	100
TOTAL		**12382.95**

Data,
09.06.2022

Dr. Dumitru-Claudiu SERGENTU,

LISTĂ DETALIATĂ

ACTIVITATEA DE CERCETARE

1. Articole științifice publicate în extenso în reviste cotate Web of Science cu factor de impact	
Total: 2786.87 puncte	
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.	(60x9.825+25)/2= **307.25**
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.	(60x4.390+25)/2= **144.20**
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.	(60x5.165+25)/11 =**30.45**
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.	(60x5.165+25)/4= **83.73**
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)	(60x5.236+25)/3= **113.05**
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.	(60x6.222+25)/13 =**30.64**
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.	(60x14.919+25)/6 =**153.36**
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.	(60x5.165+25)/7= **47.84**
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.	(60x3.376+25)/7= **32.51**
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.	(60x49.962+25)/19=**159.09**
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.	(60x3.488+25)/39 =**6.01**
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.	(60x15.336+25)/6 =**157.53**
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)	(60x5.236+25)/3= **113.05**
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)	(60x15.419+25)/15=**63.34**
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.	(60x5.165+25)/6= **55.82**
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.	(60x9.825+25)/5= **122.90**
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.	(60x15.336+25)/5 =**189.03**
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)	(60x3.676+25)/3= **81.85**

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.	(60x6.475+25)/3= **137.83**
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.	(60x14.919+25)/21=**43.82**
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.	(60x9.825+25)/3= **204.83**
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)	(60x15.419+25)/11=**86.38**
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.	(60x3.376+25)/7= **32.51**
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.	(60x4.380+25)/8= **35.98**
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.	(60x15.336+25)/7 =**135.02**
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.	(60x3.676+25)/5= **49.11**
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.	(60x3.376+25)/5= **45.51**
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.	(60x5.236+25)/12 =**28.26**
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.	(60x3.488+25)/5= **46.86**
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.	(60x3.676+25)/5= **49.11**
12. Citări și recenzii ale lucrărilor științifice (auto-citări excluse) **Reviste de specialitate din străinătate: [(20 x factor de impact + 10)/nr. autori]** **Total: 2172.95 puncte**	
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.	
1. Jun-Bo Lu, Xue-Lian Jiang, Jia-Qi Wang, Han-Shi Hu, W. H. Eugen Schwarz and Jun Li, "On the highest oxidation states of the actinoids in AnO_4 molecules (An = Ac – Cm): A DMRG-CASSCF study" J. Comput. Chem., 2022, DOI: 10.1002/jcc.26856, **IF=3.376**	**38.76**
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.	
1. Jun-Bo Lu, Xue-Lian Jiang, Jia-Qi Wang, Han-Shi Hu, W. H. Eugen Schwarz and Jun Li, "On the highest oxidation states of the actinoids in AnO_4 molecules (An = Ac-Cm): A DMRG-CASSCF study" J. Comput. Chem., 2022, DOI: 10.1002/jcc.26856**. IF=3.376**	**38.76**
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.	**0.00**
încă nu a fost citat	
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.	
1. Jun-Bo Lu, Xue-Lian Jiang, Jia-Qi Wang, Han-Shi Hu, W. H. Eugen Schwarz and Jun Li, "On the highest oxidation states of the actinoids in AnO_4 molecules (An=Ac-Cm): A DMRG-CASSCF study" J. Comput. Chem., 2022, DOI: 10.1002/jcc.26856. **IF=3.376**	**19.38**
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.	
1. Georg Poelchen, Igor P. Rusinov, Susanne Schulz, Monika Güttler, Max Mende, Alexander Generalov, Dmitry Yu. Usachov, Steffen Danzenbächer, Johannes Hellwig, Marius Peters, Kristin Kliemt, Yuri Kucherenko, Victor N. Antonov, Clemens Laubschat, Evgueni V. Chulkov,	**109.21**

	Arthur Ernst, Kurt Kummer, Cornelius Krellner, Denis V. Vyalikh, "Interlayer Coupling of a Two-Dimensional Kondo Lattice with a Ferromagnetic Surface in the Antiferromagnet $CeCo_2P_2$", *ACS Nano* 16, 3, (3573-3581), (2022). **IF=15.881**	
2.	Natalie T. Rice, Ivan A. Popov, Rebecca K. Carlson, Samuel M. Greer, Andrew C. Boggiano, Benjamin W. Stein, John Bacsa, Enrique R. Batista, Ping Yang, Henry S. La Pierre, Spectroscopic and electrochemical characterization of a Pr^{4+} imidophosphorane complex and the redox chemistry of Nd^{3+} and Dy^{3+} complexes, *Dalton Trans.* 51, 17, (6696-6706), (2022). **IF=4.390**	**32.60**
3.	Lars Hirneise, Jan Langmann, Georg Zitzer, Lukas Ude, Cäcilia Maichle-Mössmer, Wolfgang Scherer, Bernd Speiser, Reiner Anwander, "Tuning Organocerium Electrochemical Potentials by Extending Tris(cyclopentadienyl) Scaffolds with Terminal Halogenido, Siloxy, and Alkoxy Ligands", *Organometallics* 40, 11, (1786-1800), (2021). **IF=3.876**	**29.17**
4.	Laura C. Motta, Jochen Autschbach, "Theoretical Prediction and Interpretation of ^{237}Np Mössbauer Isomer Shifts", *J. Chem. Theory Comput.*, 10.1021/acs.jctc.1c00687, 17, 10, (6166-6179), (2021). **IF=6.006**	**43.37**
5.	Rulin Feng, Xiaojuan Yu, Jochen Autschbach, "Spin-Orbit Natural Transition Orbitals and Spin-Forbidden Transitions", *J. Chem. Theory Comput.*, 17, 12, (7531-7544), (2021). **IF=6.006**	**43.37**
6.	Moreau, Liane M., Ekaterina Lapsheva, Jorge I. Amaro-Estrada, Michael R. Gau, Patrick J. Carroll, Brian C. Manor, Yusen Qiao et al. "Electronic structure studies reveal 4f/5d mixing and its effect on bonding characteristics in Ce-imido and-oxo complexes." *Chem. Sci*. 13, (1759-1773), (2022). **IF=9.825**	**68.83**
7.	Bailey, Tyler A., Jennifer N. Wacker, Dahlia D. An, Korey P. Carter, Ryan C. Davis, Veronika Mocko, John Larrabee et al. "Evaluation of ^{134}Ce as a PET imaging surrogate for antibody drug conjugates incorporating 225Ac." *Nuclear Medicine and Biology* 110 (2022): 28-36. **IF=2.408**	**19.39**
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.		
încă nu a fost citat		**0.00**
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.		
1.	Ordonez, Osvaldo, Xiaojuan Yu, Guang Wu, Jochen Autschbach, and Trevor W. Hayton. "Homoleptic Perchlorophenyl "Ate" Complexes of Thorium (IV) and Uranium (IV)." Inorganic Chemistry 60, no. 16 (2021): 12436-12444. **IF=5.165**	**18.88**
2.	Réant, Benjamin LL, Victoria EJ Berryman, Annabel R. Basford, Lydia E. Nodaraki, Ashley J. Wooles, Floriana Tuna, Nikolas Kaltsoyannis, David P. Mills, and Stephen T. Liddle. "^{29}Si NMR Spectroscopy as a Probe of s-and f-Block Metal(II)-Silanide Bond Covalency." *J. Am. Chem. Soc.*, 143, no. 26 (2021): 9813-9824. **IF=15.419**	**53.06**
3.	Martel, Laura, Md Ashraful Islam, Karin Popa, Jean-Francois Vigier, Eric Colineau, Hélène Bolvin, and Jean-Christophe Griveau. "Local Structure and Magnetism of $La_{1-x}M_xPO_4$ (M= Sm, ^{239}Pu, ^{241}Am) Explained by Experimental and Computational Analyses." *The Journal of Physical Chemistry C* 125, no. 40 (2021): 22163-22174. **IF=4.126**	**15.42**
4.	Kent, Greggory T., Xiaojuan Yu, Christophe Pauly, Guang Wu, Jochen Autschbach, and Trevor W. Hayton. "Synthesis of Parent Acetylide and Dicarbide Complexes of Thorium and Uranium and an Examination of Their Electronic Structures." *Inorganic Chemistry* 60, no. 20 (2021): 15413-15420. **IF=5.165**	**18.88**
5.	Kent, Greggory T., Xiaojuan Yu, Guang Wu, Jochen Autschbach, and Trevor W. Hayton. "Synthesis and electronic structure analysis of the actinide allenylidenes, $[\{(NR_2)_3\}$ An $(CCCPh_2)]^-$ (An = U, Th; R= $SiMe_3$)." *Chemical Science*, 12, no. 43 (2021): 14383-14388. **IF=9.825**	**34.42**
6.	Kent, Greggory, Xiaojuan Yu, Guang Wu, Jochen Autschbach, and Trevor W. Hayton. "Ring-opening of a thorium cyclopropenyl complex generates a transient thorium-bound carbene", *Chemical Communications* (2022), https://doi.org/10.1039/D2CC01780F, **IF=6.222**	**22.41**
7.	Hirneise, Lars, Dennis A. Buschmann, Cäcilia Maichle-Mössmer, and Reiner Anwander. "Cerium Fluorenyl Complexes Including CC Coupling Reactions." *Organometallics*, 41, no. 8 (2022): 962-976. **IF=3.876**	**14.59**
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.		
1.	Conrad A. P. Goodwin, Michael T. Janicke, Brian L. Scott, Andrew J. Gaunt, "$[AnI_3(THF)_4]$ (An = Np, Pu) Preparation Bypassing An^0 Metal Precursors: Access to Np^{3+}/Pu^{3+} Nonaqueous and Organometallic Complexes", *J. Am. Chem. Soc.*, 2021, 143 (49), 20680-20696. **IF=15.419**	**45.48**
2.	Greggory T. Kent, Xiaojuan Yu, Christophe Pauly, Guang Wu, Jochen Autschbach, Trevor W. Hayton, "Synthesis of Parent Acetylide and Dicarbide Complexes of Thorium and Uranium and an Examination of Their Electronic Structures", *Inorg. Chem.* 2021, 60 (20), 15413-15420. **IF=5.165**	**16.19**

3. Sokratis T. Tsantis, Panagiota Danelli, Demetrios I. Tzimopoulos, Catherine P. Raptopoulou, Vassilis Psycharis, Spyros P. Perlepes, "Pentanuclear Thorium(IV) Coordination Cluster from the Use of Di(2-pyridyl) Ketone", Inorganic Chemistry 2021, 60 (16), 11888-11892. **IF=5.165**	**16.19**
4. Benjamin L. L. Réant, Victoria E. J. Berryman, Annabel R. Basford, Lydia E. Nodaraki, Ashley J. Wooles, Floriana Tuna, Nikolas Kaltsoyannis, David P. Mills, Stephen T. Liddle, "^{29}Si NMR Spectroscopy as a Probe of s- and f-Block Metal(II)-Silanide Bond Covalency", *Journal of the American Chemical Society* 2021, 143 (26), 9813-9824. **IF=15.419**	**45.48**
5. Christopher P. Gordon, Lukas Lätsch, Christophe Copéret. "Nuclear Magnetic Resonance: A Spectroscopic Probe to Understand the Electronic Structure and Reactivity of Molecules and Materials", *The Journal of Physical Chemistry Letters* 2021, 12 (8), 2072-2085. **IF=6.475**	**19.93**
6. David M. King, Benjamin E. Atkinson, Lucile Chatelain, Matthew Gregson, John A. Seed, Ashley J. Wooles, Nikolas Kaltsoyannis, Stephen T. Liddle, "Uranium-nitride chemistry: uranium-uranium electronic communication mediated by nitride bridges", *Dalton Transactions* 2022, 51 (22), 8855-8864. **IF=4.390**	**13.97**
7. Selena L. Staun, Guang Wu, Wayne W. Lukens, Trevor W. Hayton. "Synthesis of a heterobimetallic actinide nitride and an analysis of its bonding", *Chemical Science* 2021, 12 (47), 15519-15527. **IF=9.825**	**29.50**
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19. Participări la manifestări științifice **Total: 100 puncte (10 x 10 puncte)**	
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.	**10**
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.	**10**
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.	**10**

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.	**10**
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.	**10**
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.	**10**
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.	**10**
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.	**10**
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**
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.	**10**

Data,
09.06.2022

Dr. Dumitru-Claudiu SERGENTU