

Fișa de autoevaluare privind standarde minimale pe domenii ale Universității

Posturi didactice pe durată nedeterminată

ANEXA 1A

Facultatea de Chimie LECTOR UNIVERSITAR	
Standarde minimale:	1. Minim 7 articole științifice publicate în extenso în reviste internaționale, cu ISI cumulată minim 8 . 2. Autor principal la 4 articole științifice publicate în extenso în reviste internaționale cotate ISI. 3. În ultimii 5 ani să fi obținut pentru articole științifice cel puțin 25% din punctajul minimal solicitat de către comisia de Chimie din cadrul CNATDCU.
Rezultat autoevaluare:	1. Condiție îndeplinită: 37 articole științifice publicate în extenso în reviste internaționale, toate sunt cotate ISI. IF cumulată: 351.6 2. Condiție îndeplinită: autor principal la 19 articole științifice, toate fiind cotate ISI. 3. Condiție îndeplinită: 20 articole științifice publicate în ultimii 5 ani (ISI cumulată 225.3), autor principal la 9 articole în ultimii 5 ani (ISI cumulată 79.4)

Data: 29.04.2025

Asist. univ. dr. Dumitru-Claudiu Sergentu

Articole științifice publicate în extenso în reviste internaționale, cotate *Web of Science* cu factor de impact (factorii de impact, IF, Clarivate Journal Citation Reports 2023)

1. A. M. Toader, M. C. Buta, I. Humelnicu, W. Urland, M. Suta, [D.-C. Sergentu](#) (*autor corespondent), F. Cimpoesu „Ab Initio Modeling of the Photoluminescence of $\text{SrCl}_2\text{:Eu}^{2+}$ -Direct Comparison between Density Functional and Wave Function Theory-Based Approaches”, *Inorg. Chem.* **2025**, 64, 5996. **IF=4.3**
2. D. R. Russo, A. N. Gaiser, A. N. Price, [D.-C. Sergentu](#) (*prim autor cu contribuții egale), J. N. Wacker, N. Katzer, A. A. Peterson, J. A. Branson, X. Yu, S. N. Kelly, E. T. Ouellette, J. Arnold, J. R. Long, W. W. Lukens, S. J. Teat, R. J. Abergel, P. L. Arnold, J. Autschbach and S. G. Minasian, „Berkelium–carbon bonding in a tetravalent berkelocene”, *Science* **2025**, 387, 974. **IF=44.7**
3. J. A. Bronson, P. W. Smith, [D.-C. Sergentu](#), D. R. Russo, Himanshu Gupta, Corwin H. Booth, J. Arnold, E. J. Schelter, J. Autschbach and S. G. Minasian, “The counterintuitive relationship between orbital energy, orbital overlap, and bond covalency in CeF_6^{2-} and CeCl_6^{2-} ”, *J. Am. Chem. Soc.* **2024**, 146, 25640. **IF=14.4**
4. [D.-C. Sergentu](#), B. Le Guennic and R. Maurice, “The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes”, *Phys. Chem Chem. Phys.*, **2024**, 26, 6844. **IF=2.9**
5. G. Li Manni, I. F. Galván, ..., [D.-C. Sergentu](#), ..., and R. Lindh, “The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry”, *J. Chem. Theory Comput.*, **2023**, 19, 6933. **IF=5.7**
6. A. Ramanathan, J. Kaplan, [D.-C. Sergentu](#), J. A. Branson, M. Ozerov, A. I. Kolesnikov, S. G. Minasian, J. Autschbach, J. W. Freeland, Z. Jiang, M. Mourigal and H. S. La Pierre, “Chemical design of electronic and

magnetic energy scales of tetravalent praseodymium materials”, *Nature Commun.*, **2023**, 14, 3134. **IF=14.7**

7. 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 $\text{U}\equiv\text{N}$ species trapped in C_{82} fullerene cages”, *Nature Commun.*, **2022**, 13, 7192. **IF=14.7**
8. [D.-C. Sergentu](#) and J. Autschbach, “Covalency in actinide(IV) hexachlorides in relation to chlorine K-edge X-ray absorption structure”, *Chem. Sci.* **2022**, 13, 3194. **IF=7.6**
9. [D.-C. Sergentu](#) and J. Autschbach, “X-ray absorption spectra of f-element complexes: Insight from relativistic multiconfigurational wavefunction theory”, *Dalton Trans.*, **2022**, 51, 1754. **IF=3.5**
10. [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: $\text{Cs}_2\text{UO}_2\text{Cl}_4$ and $\text{Cs}_2\text{UO}_2\text{Br}_4$ ”, *Inorg. Chem.* **2022**, 61, 3821. **IF=4.3**
11. 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.*, **2021**, 60, 17744. **IF=4.3**
12. [D.-C. Sergentu](#) (*[autor corespondent](#)), C. Booth and J. Autschbach, “Probing multiconfigurational states by spectroscopy: The cerium XAS L3-edge puzzle”, *Chem. Eur. J.*, **2021**, 27, 7239. **IF=3.9**
13. 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 $[\text{U}(\text{C}_7\text{H}_7)_2]^-$: C K-edge XAS, magnetism, and ab initio calculations”, *Chem. Commun.*, **2021**, 57, 9562. **IF=4.3**
14. 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.* **2021**, 12, 1713. **IF=14.7**
15. [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.* **2020**, 59, 10138. **IF=4.3**
16. 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.* **2020**, 41, 2055. **IF=3.4**
17. 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* **2020**, 583, 396. **IF=50.5**
18. 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. Odellius, 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.* **2020**, 152, 214117. **IF=3.1**
19. 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.*, **2020**, 59, 13586. **IF=16.1**
20. G. Ganguly, [D.-C. Sergentu](#) (*[prim autor cu contribuții egale](#)), and J. Autschbach, “Ab initio analysis of metal-ligand bonding in $\text{An}(\text{COT})_2$ with $\text{An} = \text{Th}, \text{U}$ in their ground and core-excited states”, *Chem. Eur. J.*, **2020**, 26, 1776. **IF=3.9**
21. J. Zhuang, L. Abella, [D.-C. Sergentu](#) (*[prim autor cu contribuții egale](#)), 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.* **2019**, 141, 20249. **IF=14.4**
22. 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.* **2019**, 58, 12654. **IF=4.3**
23. 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.* **2019**, 10, 6431. **IF=7.6**
24. N. J. Wolford, [D.-C. Sergentu](#), W. Brennessel, J. Autschbach and M. Neidig, "Homoleptic aryl complexes of uranium(IV)", *Angew. Chem. Int. Ed.* **2019**, 58, 10266. **IF=16.1**
25. Y. Heit, [D.-C. Sergentu](#) (*prim autor cu contribuții egale) and J. Autschbach, "Magnetic circular dichroism spectra of transition metal complexes calculated from restricted active space wavefunctions", *Phys. Chem. Chem. Phys.* **2019**, 21, 5586. **IF=2.9**
26. [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.* **2018**, 9, 5583. **IF=4.8**
27. 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.* **2018**, 9, 2753. **IF=14.7**
28. [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.* **2018**, 9, 6292. **IF=7.6**
29. Y. Quao, [D.-C. Sergentu](#) (*prim autor cu contribuții egale), 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.* **2018**, 140, 4588. **IF=14.4**
30. 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.* **2017**, 38, 2753. **IF=3.4**
31. 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.* **2017**, 7, 2579. **IF=3.8**
32. 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.*, **2016**, 55, 15369. **IF=16.1**
33. [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.* **2016**, 18, 32703. **IF=2.9**
34. [D.-C. Sergentu](#), G. David, G. Montavon, R. Maurice and N. Galland, "Scrutinizing "invisible" astatine: A challenge for modern density functionals", *J. Comput. Chem.* **2016**, 37, 1345. **IF=3.4**
35. [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.* **2016**, 22, 2964. **IF=3.9**
36. [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.* **2015**, 143, 114306. **IF=3.1**
37. [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.* **2014**, 16, 25393. **IF=2.9**

ANEXA 1

Fișă de autoevaluare Alcatuită în conformitate cu prevederile fișei de evaluare generală a standardelor Universității

A. ACTIVITATEA DE CERCETARE	
DESCRIPTORI	PUNCTAJ
1. Articole științifice publicate <i>in extenso</i> în reviste cotate <i>Web of Science</i> cu factor de impact	2947.199
2. Contracte de cercetare științifică	1.487
3. Citări și recenzii ale lucrărilor științifice (<i>doar ptr. ultimele 10 articole</i>)	20796.798
4. Premii și distincții la nivel național	20
5. Participări la manifestări științifice	130
TOTAL A	23895.484
B. ACTIVITATEA DIDACTICĂ	
DESCRIPTORI	PUNCTAJ
1. Materiale suport curs, seminar, lucrări practice și programe analitice detaliate	50
2. Evaluarea gradului de îndeplinire a unor obiective specifice, stabilite în acord cu misiunea și obiectivele Universității, ale facultății sau departamentului	30
TOTAL B	80

Data

29.04.2025

Asist. univ. dr. Dumitru-Claudiu SERGENTU

ACTIVITATEA DE CERCETARE

Nr. crt.	Descriptor	Punctaj
1.	Articole științifice publicate in extenso în reviste cotate Web of Science cu factor de impact (Metoda de calcul: (60 puncte x factor de impact + 25) / număr autori)	
	1. (7 autori) Toader, AM; Buta, MC; Humelnicu, I; Urland, W; Suta, M; Sergentu, DC ; Cimpoesu, F, Ab Initio Modeling of the Photoluminescence of SrCl ₂ :Eu ²⁺ -Direct Comparison between Density Functional and Wave Function Theory-Based Approaches, INORGANIC CHEMISTRY, 64, 5996-6009, , 2025, IF: 4.3	40.429
	2. (19 autori) Russo, DR; Gaiser, AN; Price, AN; Sergentu, DC ; Wacker, JN; Katzer, N; Peterson, AA; Branson, JA; Yu, XJ; Kelly, SN; Ouellette, ET; Arnold, J; Long, JR; Lukens, WW Jr; Teat, SJ; Abergel, RJ; Arnold, PL; Autschbach, J; Minasian, SG, Berkelium-carbon bonding in a tetravalent berkelocene, SCIENCE, 387, 974-978, , 2025, IF: 44.7	142.474
	3. (10 autori) Branson, JA; Smith, PW; Sergentu, DC ; Russo, DR; Gupta, H; Booth, CH; Arnold, J; Schelter, EJ; Autschbach, J; Minasian, SG, The Counterintuitive Relationship between Orbital Energy, Orbital Overlap, and Bond Covalency in CeF ₆ 2- and CeCl ₆ 2-, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 146, 25640-25655, , 2024, IF: 14.4	88.900
	4. (3 autori) Sergentu, DC ; Le Guennic, B; Maurice, R, The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 26, 6844-6861, , 2024, IF: 2.9	66.333
	5. (12 autori) Ramanathan, A; Kaplan, J; Sergentu, DC ; Branson, JA; Ozerov, M; Kolesnikov, AI; Minasian, SG; Autschbach, J; Freeland, JW; Jiang, ZG; Mourigal, M; La Pierre, HS, Chemical design of electronic and magnetic energy scales of tetravalent praseodymium materials, NATURE COMMUNICATIONS, 14, -, 3134, 2023, IF: 14.7	75.583
	6. (108 autori) Manni, GL; Galván, IF; Alavi, TR; ...; Sergentu, DC ; Sharma, P; Shepard, R; Shu, YN; Staab, JK; Straatsma, TP; Sorensen, LK; Tenorio, BNC; Truhlar, DG; Ungur, L; Vacher, M; Veryazov, V; Voss, TA; Weser, O; Wu, DH; Yang, XC; Yarkony, D; Zhou, C; Zobel, JP; Lindh, R, The OpenMolcas Web: A Community-Driven Approach to Advancing Computational Chemistry, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 19, 6933-6991, , 2023, IF: 5.7	3.398
	7. (10 autori) Meng, QY; Abella, L; Yao, YR; Sergentu, DC ; Yang, W; Liu, XY; Zhuang, JX; Echegoyen, L; Autschbach, J; Chen, N, A charged diatomic triple-bonded U≡N species trapped in C ₈₂ fullerene cages, NATURE COMMUNICATIONS, 13, -, 7192, 2022, IF: 14.7	90.700
	8. (11 autori) Sergentu, DC ; Gendron, F; Walter, ED; Park, S; Capan, C; Surbella, RG; Soderquist, CZ; Hall, GB; Sinkov, SI; Autschbach, J; Cho, H, Equatorial Electronic Structure in the Uranyl Ion: Cs ₂ UO ₂ Cl ₄ and Cs ₂ UO ₂ Br ₄ , INORGANIC CHEMISTRY, 61, 3821-3831, , 2022, IF: 4.3	25.727
	9. (2 autori) Sergentu, DC ; Autschbach, J, Covalency in actinide(IV) hexachlorides in relation to the chlorine K-edge X-ray absorption structure, CHEMICAL SCIENCE, 13, 3194-3207, , 2022, IF: 7.6	240.500

10. (2 autori) Sergentu, DC ; Autschbach, J, X-ray absorption spectra of f-element complexes: insight from relativistic multiconfigurational wavefunction theory, DALTON TRANSACTIONS, 51, 1754-1764, , 2022, IF: 3.5	117.500
11. (4 autori) Yu, XJ; Sergentu, DC ; Feng, RL; Autschbach, J, Covalency of Trivalent Actinide Ions with Different Donor Ligands: Do Density Functional and Multiconfigurational Wavefunction Calculations Corroborate the Observed Breaks?, INORGANIC CHEMISTRY, 60, 17744-17757, , 2021, IF: 4.3	70.750
12. (13 autori) Qiao, YS; Ganguly, G; Booth, CH; Branson, JA; Ditter, AS; Lussier, DJ; Moreau, LM; Russo, DR; Sergentu, DC ; Shuh, DK; Sun, TX; Autschbach, J; Minasian, SG, Enhanced 5f- δ bonding in [U(C ₇ H ₇) ₂]-: C K-edge XAS, magnetism, and ab initio calculations, CHEMICAL COMMUNICATIONS, 57, 9562-9565, , 2021, IF: 4.3	21.769
13. (7 autori) Panetti, GB; Sergentu, DC ; Gau, MR; Carroll, PJ; Autschbach, J; Walsh, PJ; Schelter, EJ, Isolation and characterization of a covalent CeIV- Aryl complex with an anomalous ¹³ C chemical shift, NATURE COMMUNICATIONS, 12, -, 1713, 2021, IF: 14.7	129.571
14. (3 autori) Sergentu, DC ; Booth, CH; Autschbach, J, Probing Multiconfigurational States by Spectroscopy: The Cerium XAS L3-edge Puzzle, CHEMISTRY-A EUROPEAN JOURNAL, 27, 7239-7251, , 2021, IF: 3.9	86.333
15. (7 autori) Sergentu, DC ; Kent, GT; Staun, SL; Yu, XJ; Cho, H; Autschbach, J; Hayton, TW, Probing the Electronic Structure of a Thorium Nitride Complex by Solid-State ¹⁵ N NMR Spectroscopy, INORGANIC CHEMISTRY, 59, 10138-10145, , 2020, IF: 4.3	40.429
16. (19 autori) Sperling, JM; Warzecha, EJ; Celis-Barros, C; Sergentu, DC ; Wang, XY; Klamm, BE; Windorff, CJ; Gaiser, AN; White, FD; Beery, DA; Chemey, AT; Whitefoot, MA; Long, BN; Hanson, K; Koegerler, P; Speldrich, M; Zurek, E; Autschbach, J; Albrecht-Schonzart, TE, Compression of curium pyrrolidine-dithiocarbamate enhances covalency, NATURE, 583, 396-, , 2020, IF: 50.5	160.789
17. (7 autori) Pech, CG; Haase, PAB; Sergentu, DC ; Borschevsky, A; Pilmé, J; Galland, N; Maurice, R, Quantum chemical topology at the spin-orbit configuration interaction level: Application to astatine compounds, JOURNAL OF COMPUTATIONAL CHEMISTRY, 41, 2055-2065, e26373, 2020, IF: 3.4	32.714
18. (39 autori) Aquilante, F; Autschbach, J; Baiardi, A; Battaglia, S; Borin, VA; Chibotaru, LF; Conti, I; De Vico, L; Delcey, M; Galvan, IF; Ferré, N; Freitag, L; Garavelli, M; Gong, XJ; Knecht, S; Larsson, ED; Lindh, R; Lundberg, M; Malmqvist, PÅ; Nenov, A; Norell, J; Odelius, M; Olivucci, M; Pedersen, TB; Pedraza-González, L; Phung, QM; Pierloot, K; Reiher, M; Schapiro, I; Segarra-Martí, J; Segatta, F; Seijo, L; Sen, S; Sergentu, DC ; Stein, CJ; Ungur, L; Vacher, M; Valentini, A; Veryazov, V, Modern quantum chemistry with [Open]Molcas, JOURNAL OF CHEMICAL PHYSICS, 152, -, , 2020, IF: 3.1	5.410
19. (6 autori) Sears, JD; Sergentu, DC ; Baker, TM; Brennessel, WW; Autschbach, J; Neidig, ML, The Exceptional Diversity of Homoleptic Uranium-Methyl Complexes,	165.167

	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 59, 13586-13590, , 2020, IF: 16.1	
	20. (3 autori) Ganguly, G; Sergentu, DC ; Autschbach, J, Ab Initio Analysis of Metal-Ligand Bonding in An(COT) ₂ with An=Th, U in Their Ground- and Core-Excited States, CHEMISTRY-A EUROPEAN JOURNAL, 26, 1776-1788, , 2020, IF: 3.9	86.333
	21. (15 autori) Zhuang, JX; Abella, L; Sergentu, DC ; Yao, YR; Jin, MH; Yang, W; Zhang, XX; Li, XM; Zhang, D; Zhao, YM; Li, XH; Wang, S; Echegoyen, L; Autschbach, J; Chen, N, Diuranium(IV) Carbide Cluster U ₂ C ₂ Stabilized Inside Fullerene Cages, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 141, 20249-20260, , 2019, IF: 14.4	59.267
	22. (6 autori) Assefa, MK; Sergentu, DC ; Seaman, LA; Wu, G; Autschbach, J; Hayton, TW, Synthesis, Characterization, and Electrochemistry of the Homoleptic f Element Ketimide Complexes [Li] ₂ [M(N=CtBuPh) ₆] (M = Ce, Th), INORGANIC CHEMISTRY, 58, 12654-12661, , 2019, IF: 4.3	47.167
	23. (5 autori) Wolford, NJ; Sergentu, DC ; Brennessel, WW; Autschbach, J; Neidig, ML, Homoleptic Aryl Complexes of Uranium (IV), ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 58, 10266-10270, , 2019, IF: 16.1	198.200
	24. (5 autori) Staun, SL; Sergentu, DC ; Wu, G; Autschbach, J; Hayton, TW, Use of 15N NMR spectroscopy to probe covalency in a thorium nitride, CHEMICAL SCIENCE, 10, 6431-6436, , 2019, IF: 7.6	96.200
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	Subtotal 2	1.487
3.	Citări și recenzii ale lucrărilor științifice	
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27. Bignon, E; Marazzi, M; Besancenot, V; Gattuso, H; Drouot, G; Morell, C; Eriksson, LA; Grandemange, S; Dumont, E; Monari, A, Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process, SCIENTIFIC REPORTS, 7, -, 8885, 2017, IF: 3.8	17.200
28. Francés-Monerris, A; Galván, IF; Lindh, R; Roca-Sanjuán, D, Triplet versus singlet chemiexcitation mechanism in dioxetanone: a CASSCF/CASPT2 study, THEORETICAL CHEMISTRY ACCOUNTS, 136, -, 70, 2017, IF: 1.6	8.400
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31. Dormán, G; Nakamura, H; Pulsipher, A; Prestwich, GD, The Life of Pi Star: Exploring the Exciting and Forbidden Worlds of the Benzophenone Photophore, CHEMICAL REVIEWS, 116, 15284-15398, , 2016, IF: 51.4	207.600
32. Soep, B; Mestdagh, JM; Briant, M; Gaveau, MA; Poisson, L, Direct observation of slow intersystem crossing in an aromatic ketone, fluorenone, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 18, 22914-22920, , 2016, IF: 2.9	13.600
33. Vlaisavljevich, B; Shiozaki, T, Nuclear Energy Gradients for Internally Contracted Complete Active Space Second-Order Perturbation Theory: Multistate Extensions, JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 12, 3781-3787, , 2016, IF: 5.7	24.800
34. Favero, L; Granucci, G; Persico, M, Surface hopping investigation of benzophenone excited state dynamics, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 18, 10499-10506, , 2016, IF: 2.9	13.600
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	39. Liu, LZ; Pilles, BM; Reiner, AM; Gontcharov, J; Zinth, W, 2'-Methoxyacetophenone: An Efficient Photosensitizer for Cyclobutane Pyrimidine Dimer Formation, CHEMPHYSCHEM, 16, 3483-3487, , 2015, IF: 2.3	11.200
	40. Huix-Rotllant, M; Dumont, E; Ferré, N; Monari, A, Photophysics of Acetophenone Interacting with DNA: Why the Road to Photosensitization is Open, PHOTOCHEMISTRY AND PHOTOBIOLOGY, 91, 323-330, , 2015, IF: 2.6	12.400
	41. Ouyang, WJ; Dou, WJ; Subotnik, JE, Surface hopping with a manifold of electronic states. I. Incorporating surface-leaking to capture lifetimes, JOURNAL OF CHEMICAL PHYSICS, 142, -, 84109, 2015, IF: 3.1	14.400
	42. Dumont, E; Wibowo, M; Roca-Sanjuán, D; Garavelli, M; Assfeld, X; Monari, A, Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level, JOURNAL OF PHYSICAL CHEMISTRY LETTERS, 6, 576-580, , 2015, IF: 4.8	21.200
	Subtotal 3	20796.798
4.	Alte premii naționale ale instituțiilor culturale (Metoda de calcul: 20 puncte / categorie / număr persoane)	
	1. Premiul I în competiția “Tineri cercetători în știință și inginerie”, desemnat cel mai bun cercetător din România cu vârsta sub 35 ani, ediția a X-a a premiilor „Rada Mihalcea pentru Tineri Cercetători în Știință și Inginerie” 27 Iunie 2024, premiul oferit de primăria Cluj-Napoca în colaborare cu Prof. univ. Rada Mihalcea (Universitatea Michigan, SUA), Cluj-Napoca, România. https://primariaclužnapoca.ro/evenimente/tinerii-cercetatori-premiul-pentru-stiinta-si-inginerie/	20
	Subtotal 4	20.000
5.	Participări la manifestări științifice	
	Internaționale – raportor pe secțiuni/paneluri (Metoda de calcul: pentru fiecare activitate 10 puncte)	
	1. D.-C. Sergentu , I. Humelnicu și J. Autschbach, Tetravalent cerium coordination: Understanding the L3-edge X-ray absorption structure in organocerium complexes, CoFRO: Coordination Chemistry between France and Romania, 15–16 Mai, 2024, Rennes, Franța. (prezentare orală).	10.000
	2. D.-C. Sergentu , B. Le Guennic, R. Maurice, Simple resolution of the standard multispin Hamiltonian in the weak exchange regime, Journées de l'Association française de Magnétisme Moléculaire (JAM2-2023), 13–16 Noiembrie, 2024, Mittelwihr, Franța. (prezentare orală).	10.000
	3. D.-C. Sergentu , B. Le Guennic and R. Maurice, The resolution of the weak-exchange limit made rigorous, simple and general in binuclear complexes: A theoretical feat, 17th International Congress of Quantum Chemistry (ICQC2023), 26 Mai – 1 Iunie 2023, Bratislava, Slovacia. (prezentare orală).	10.000

4.	D.-C. Sergentu , B. Le Guennic, R. Maurice, Simple resolution of the standard multispin Hamiltonian in binuclear complexes, International Conference of Physical Chemistry (ROMPHYSICHEM 17), 25-27 Septembrie 2023, București, Romania. (prezentare orală)	10.000
5.	D.-C. Sergentu , I. Humelnicu și J. Autschbach, Insights Into Electronic Structure and Metal-Ligand Bonding in f-Element Systems Through Computational X-ray Absorption Spectroscopy, PolyChar World Forum on Advanced Materials (POLY CHAR'30), 11-13 Septembrie 2024, Iasi, Romania (prezentare orală).	10.000
6.	D.-C. Sergentu „Electronic structure and metal-ligand bonding in tetravalent cerium complexes: Computational chemistry experiments”, Recent Advances in Natural Sciences Yield the Future for the European Citizens and Society, Universitatea „Alexandru Ioan Cuza” din Iași, Iași, Romania, 12-13 December 2024. (prezentare orală)	10.000
7.	D.-C. Sergentu “NewMag: New tools for the rational design of single molecule Magnets by model and effective Hamiltonian approaches”, European Responsible Research and Innovation Event 2023 (ERRIE 2023), Brest, France, 10-11 May 2023. (poster)	10.000
8.	D.-C. Sergentu and J. Autschbach, “X-ray absorption spectroscopy: Chemical bonding in actinide complexes from ab initio multireference wavefunction approaches”, 2nd European Symposium on Chemical Bonding, Oviedo, Spain, 3–7 September, 2018. (poster)	10.000
9.	D.-C. Sergentu , F. Réal, N. Galland and R. Maurice, “The peculiar electronic structure of AtO ⁺ in water”, 7th International Meeting on Atomic and Molecular Physics and Chemistry, Le Havre, France, 27–30 June, 2016. (poster)	10.000
10.	D.-C. Sergentu , N. Galland and R. Maurice, “Ground-state reversal induced by solvation: Electronic structure of AtO ⁺ in water”, TALISMAN ThUL School in Actinide Chemistry, Karlsruhe, Germany, 28 September-2 October, 2015. (poster)	10.000
11.	D.-C. Sergentu , N. Galland and R. Maurice, “Electronic structures of the XF ₃ (X = Cl, Br, I, At) fluorides and topology of their potential energy surfaces”, 2nd European Symposium on Density Functional Theory and its Applications, Debrecen, Hungary, 31 August-4 September, 2015. (prezentare orală)	10.000
12.	D.-C. Sergentu , J. Champion, A. Sabatié-Gogova, J.-Y. Le Questel, R. Maurice, G. Mon- tapon and N. Galland, “Investigation of the AtO(OH)–hydrolysed species: Relativistic calculations”, SOSTRUP Summer School : Quantum Chemistry and Molecular Properties, Himmelbjergettegnens Natur-og Idrætsefterskole, Denmark, 6–18 July, 2014. (poster)	10.000

13. D.-C. Sergentu , D. Roca-Sanjuán, R. W. A. Havenith and R. Braam-Broer, “Revisiting the intersystem crossing in benzophenone”, 9th European Conference on Computational Chemistry, Sopron, Hungary, 2–6 September, 2013. (prezentare orală)	10.000
Subtotal 5	130.000
TOTAL A ACTIVITATEA DE CERCETARE	23895.484

B ACTIVITATEA DIDACTICĂ

Nr. crt.	Descriptor	Punctaj
1.	Materiale suport curs, seminar, lucrări practice și programe analitice detaliate Metoda de calcul: 10 puncte pentru fiecare activitate)	
	1. Chimie cuantică și structură, an II studii de licență	10
	2. Chimie medicală computațională și structurală, an II studii de licență	10
	3. Chimie computațională și termodinamică statistică (op), an III studii de licență	10
	4. Modelarea structurii moleculare și transport prin membrane (op), an III studii de licență	10
	5. Structura, dinamica și energetica sistemelor moleculare. Farmacocinetică și farmacodinamică (op), an II studii de master	10
	Subtotal 1	50
2.	Evaluarea gradului de îndeplinire a unor obiective specifice, stabilite în acord cu misiunea și obiectivele Universității, ale facultății sau departamentului a. inițierea, conducerea sau participarea la elaborarea și derularea unor programe și activități de interes major pentru Universitate sau facultate	
	1. Membru în comitetul de organizare a sesiunii de comunicări științifice a studenților, masteranzilor și doctoranzilor din 27 iunie 2024 (SCSSMD, ediția a XV-a, Chimia – Frontieră Deschisă spre Cunoaștere), link aici .	5
	2. Membru în comisia de admitere pentru Facultatea de Chimie, sesiunea 2025-2026.	15
	b. contribuții specifice la realizarea misiunii și obiectivelor Universității, facultății sau departamentului	
	1. Membru în comisia de supraveghere pentru concursul de Chimie “Magda Petrovanu”, sesiunea 2024.	10
	Subtotal 2	30
	TOTAL B ACTIVITATEA DIDACTICĂ	80

Data

29.04.2025

Asist. univ. dr. Sergentu Dumitru-Claudiu

Semnătură: _____