Fișa de verificare

a îndeplinirii criteriilor de abilitare

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Funcţia actuală: Conferential universitar
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Criterii CNATDCU – Criterii Abilitare domeniul CHIMIE

	Criterii minimale CNATDCU	Punctaj realizat
N_{max}	50	50
FIC	100	189,7
FIC_D	70	180,3
FIC_{AP}	50	101,0
FIC_{AC}	25	86,2
H index	13	15 Clarivate 16 Scopus

N_{max} – primele maxim N lucrari

FIC – fact de impact cumulat

FIC_D – factor de impact cumulat domeniu

FIC_{AP} – factor de impact cumulat autor principal (prim-autor și autor de corespondență)

FIC_{AP} – factor de impact cumulat autor de corespondență

În continuare este prezentată lista celor 50 de publicații Nmax în ordinea descrescătoare a factorilor de impact, așa cum sunt ei raportați în ISI Web of knowledge.

1. "Unusual dimetallaborane cluster polyhedra and their skeletal bonding" A. Lupan*, A.A. Attia, R.B. King, *Coord. Chem. Rev.*, 2017, *345*, 1-5; doi:10.1016/j.ccr.11001 (c. 2, F.I. 20,3)
2. "New class of hybrid materials for detection, capture and on-demand release of carbon monoxide" A. Pitto-Barry, A. Lupan, C. Ellingford, A.A. Attia, N.P. Barry, *ACS Appl. Mater. Interfaces*, 2018, *10*, 13693-13701; doi: 10.1021/acsami.8b01776 (c. 9, F.I. 8,5)
3. "First-in-class allosteric inhibitors of bacterial IMPDHs" T. Alexandre, A. Lupan, O. Helynck, S. Vichier-Guerre, L. Dugue, M. Gelin, A. Haouz, G. Labesse, H. Munier-Lehmann, *Eur. J. Med. Chem.*, 2019, *167*, 124-132; doi: 10.1016/j.ejmech.2019.01.064 (c. 11, F.I. 6,0)
4. "Inhibition of pyrimidine biosynthesis pathway suppresses viral growth through innate immunity" M. Lucas-Hourani, D. Dauzonne, P. Jorda, G. Cousin, A. Lupan et.al., *Plos Pathog.*, 2013, 9, e1003678. doi: 10.1371/journal.ppat.1003678 (c. 119, F.I. 5,5)
5. "Nonspherical deltahedra in low-energy dicarbalane structures testing the Wade–Mingos rules: the regular icosahedron is not favored for the 12-vertex dicarbalane" A.A. Attia, A. Lupan*, R.B. King, *Inorg. Chem.*, 2015, *54*, 11377-11384; doi:10.1021/ acs.inorgchem.5b02014 (c. 10, F.I. 4,3)

6. "Triplet spin-state capped deltahedral structures rather than singlet spin-state oblatocloso structures as energetically favored dimanganaborane structures" A. Gaina-Gardiuta, A. Lupan*, R.B. King, *Inorg. Chem.*, 2022, *61*, 20793-20803; doi: 10.1021/inorgchem.2c02936 (F.I. 4,3)
7. "Spherical closo deltahedra with surface metal-metal multiple bonding versus oblate deltahedra with internal metal-metal bonding in dichromadicarbaborane structures: the nature of Stone's icosahedral dichromadicarbaborane" S. Jákó, A. Lupan*, A.Z. Kun, R.B. King, *Inorg. Chem.*, 2019, *58*, 3825-3837; doi: 10.1021/acs.inorgchem.8b03476 (c. 1, F.I. 4,3)
8. "Hypoelectronicity and chirality in dimetallaboranes of the group 9 metals cobalt, rhodium, and iridium" S. Jákó, A. Lupan*, A.Z. Kun, R.B. King, *Inorg. Chem.*, 2017, *56*, 351-358; doi: 10.1021/acs.inorgchem.6b02281 (c. 1, F.I. 4,3)
9. "Paramagnetism in metallacarboranes: the polyhedral chromadicarbaborane systems" S. Jákó, A. Lupan*, A.Z. Kun, R.B. King, *Inorg Chem*, 2017, *56*, 11059-11065; doi: 10.1021/acs.inorgchem.7b01422 (c. 1, F.I. 4,3)
10. "Deviations from the most spherical deltahedra in rhenatricarbaboranes having 2n + 2 wadean skeletal electrons" A.A. Attia, A. Lupan*, R.B. King, *Inorg. Chem.*, 2017, *56*, 15015-15025; doi: 10.1021/acs.inorgchem.7b02348 (c. 2, F.I. 4,3)
11. "Magnesium(II) D-gluconate complexes relevant to radioactive waste disposals: metal ion-induced ligand deprotonation or ligand-promoted metal ion hydrolysis?" B Kutus, C. Dudás, Csilla, E. Orban, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, G. Peintler, *Inorg Chem*, 2019, *58*, 6832-6844; doi: 10.1021/acs.inorgchem.9b00289 (c. 9, F.I. 4,3)
12. "Density functional theory study of 11-atom germanium clusters: Effect of electron count on cluster geometry" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, *Inorg. Chem.*, 2005, *44*, 3579; doi: 10.1021/ic040110x (c. 31, F.I. 4,3)
13. "Hypoelectronic dirhenaboranes having eight to twelve vertices: internal versus surface rhenium-rhenium bonding" A. Lupan, R.B. King, *Inorg. Chem.*, 2012, *51*, 7609; doi: 10.1021/ic300458w (c. 26, F.I. 4,3)
14. "Limited occurrence of isocloso deltahedra with 9 to 12 vertices in low-energy hypoelectronic diferradicarbaborane structures" A. Lupan, R.B. King, *Inorg. Chem.*, 2011, *50*, 9571; doi: 10.1021/ic201321f (c. 24, F.I. 4,3)
15. "Density functional study of 8-and 11-vertex polyhedral borane structures: Comparison with bare germanium clusters" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, *Inorg. Chem.*, 2005, *44*, 7819; doi: 10.1021/ic050656z (c. 10, F.I. 4,3)
16. "Microwave assisted synthesis, photophysical and redox properties of (phenothiazinyl) vinyl-pyridinium dyes" L. Gainã, I. Torje, E. Gal, A. Lupan, C. Bischin, R. Silaghi-Dumitrescu, G. Damian, P. Lonnecke, C. Cristea, L. Silaghi-Dumitrescu, *Dyes Pigm.*, 2014, 102, 315-325; doi: 10.1016/j.dyepig.2013.10.044 (c. 23, F.I. 4,1)
17. "Spin state preference and bond formation/cleavage barriers in ferrous-dioxygen heme adducts: remarkable dependence on methodology" A.A. Attia, A. Lupan, R. Silaghi-Dumitrescu, *RSC Adv.*, 2013, *3*, 26194-26204; doi: 10.1039/C3RA45789C (c. 20, F.I. 3,9)
18. "Electromerism and linkage isomerism in biologically-relevant Fe-SO complexes" M. Surducan, D. Lup, A. Lupan, S. Makarov, R. Silaghi-Dumitrescu, *J. Inorg. Biochem.*, 2013, *118*, 13; doi: 10.1016/j.jinorgbio.2012.09.013 (c. 13, F.I. 3,8)
19. "Multiconfigurational and DFT analyses of the electromeric formulation and UV-Vis absorption spectra of the superoxide adduct of ferrous superoxide reductase" A.A. Attia, D. Cioloboc, A. Lupan, R. Silaghi-Dumitrescu, *J. Inorg. Biochem.*, 2016, *165*, 49-53; doi: 10.1016/j.jinorgbio.2016.09.017 (c. 11, F.I. 3,8)
20. "Synergy of the antibiotic colistin with echinocandin antifungals in Candida species" U. Zeidler, M.E. Bougnoux, A. Lupan, O. Helynck, A. Doyen, Z. Garcia, N. Sertour, C. Clavaud, H. Munier-Lehmann, C. Saveanu, C. d'Enfert, *J. Antimicrob. Chemother.*, 2013, *68*, 1285; doi: 10.1093/jac/dks538 (c. 47, F.I. 3,9)

21. "Reversible complexation of ammonia by breaking a manganese-manganese bond in a manganese carbonyl ethylenedithiolate complex: A theoretical study of an unusual type of Lewis acid" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan*, R.B. King, *Dalton Trans.*, 2019, *48*, 324-332; doi: 10.1039/C8DT04217A (c. 2, F.I. 3,5)
22. "Deltahedral ferratricarbaboranes: analogues of ferrocene" A. Lupan*, R.B. King, *Dalton Trans.*, 2014, *43*, 4993-5000; doi: 10.1039/C3DT52381K (c. 9, F.I. 3,5)
23. "Tetracarbalane structures: nido polyhedra and non-spherical deltahedra" A.A. Attia, A. Lupan*, R.B. King, *Dalton Trans.*, 2016, *45*, 11528-11539; doi: 10.1039/c6dt01982j (c. 4, F.I. 3,5)
24. "Tetracarbaboranes: nido structures without bridging hydrogens" A.A. Attia, A. Lupan, R.B. King, *Dalton Trans.*, 2016, *45*, 18541-18551; doi: 10.1039/C6DT03507H (c. 1, F.I. 3,5)
25. "Dimetallaborane analogues of pentaborane" A.M.V. Branzanic, A. Lupan*, R.B. King, *Dalton Trans.*, 2015, *44*, 7355-7363; doi: 10.1039/C5DT00143A (c. 2, F.I. 3,5)
26. "Density functional theory study of eight-atom germanium clusters: Effect of electron count on cluster geometry" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, *Dalton Trans.*, 2005, *10*, 1858; doi: 10.1039/b501855b (c. 26, F.I 3,5)
27. "The prevalence of isocloso deltahedra in low-energy hypoelectronic metalladicarbaboranes with a single metal vertex: manganese and rhenium derivatives" A. Lupan, R.B. King, *Dalton Trans.*, 2012, *41*, 7073; doi: 10.1039/c2dt30442b (c. 13, F.I. 3,5)
28. "Pseudo electron-deficient organometallics: limited reactivity towards electron-donating ligands" A. Pitto-Barry, A. Lupan, M. Zegke, T. Swift, A.A. Attia, R.M. Lord, N.P. Barry, *Dalton Trans.*, 2017, *46*, 15676-15683; doi: 10.1039/C7DT02827J (c. 14, F.I. 3,5)
29. "Formation of mono and binuclear neodymium(III)-gluconate complexes in aqueous solutions in the pH range of 2-8" B. Kutus, N. Varga, G. Peintler, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, *Dalton Trans.*, 2017, *46*, 6049-6058; doi: 10.1039/C7DT00909G (c. 13, F.I. 3,5)
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31. "On the roles of alanine and serine in the β-sheet structure of fibroin" J.F. Carrascoza Mayen, A. Lupan, C. Cosar, A.Z. Kun, R. Silaghi-Dumitrescu, *Biophys. Chem.*, 2015, *197*, 10-17; doi:10.1016/j.bpc.2014.11.001 (c. 11, F.I. 3,3)
32. "The tetracapped truncated tetrahedron in 16-vertex tetrametallaborane structures: spherical aromaticity with an isocloso rather than a closo skeletal electron count" A.A. Attia, A. Lupan*, R.B. King, S. Ghosh, *Phys. Chem. Chem. Phys.*, 2019, *21*, 22022-22030; doi: 10.1039/c9cp04263f (c. 5, F.I. 2,9)
33. "Cationic gold clusters with eight valence electrons: possible spherical aromatic systems with sigma holes" A.A. Attia, A. Branzanic, A. Muñoz-Castro, A. Lupan*, R.B. King, *Phys. Chem. Chem. Phys.*, 2019, *21*, 17779-17785; doi: 10.1039/C9CP03440D (c. 5, F.I. 2,9)
34. "Biicosahedral metallaboranes: aromaticity in metal derivatives of three-dimensional analogues of naphthalene" A.A. Attia, A. Lupan*, R.B. King, *Phys. Chem. Chem. Phys.*, 2016, *18*, 11707-11710; doi: 10.1039/c5cp05708f (c. 3, F.I. 2,9)
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36. "Fe-O versus O-O bond cleavage in reactive iron peroxide intermediates of superoxide reductase" A. Attia, D. Cioloboc, A. Lupan, R. Silaghi-Dumitrescu, *J. Biol. Inorg. Chem.*, 2013, *18*, 95; doi: 10.1007/s00775-012-0954-4 (c. 12, F.I. 2,7)

37. "Iron carbonyl complexes of a rigid chelating dicarbene: a density functional theory study" C. Balaiu, A.A. Attia, A. Lupan*, R.B. King, *Inorg. Chim. Acta*, 2021*, 514,* 120002; doi: 10.1016/j.ica.2020.120002 (c. 4, F.I. 2,7)
38. "Metal–metal interactions in deltahedral dirhoda- and diiridadicarbaboranes" A. Lupan, R.B. King, *Inorg. Chim. Acta*, 2013, *397*, 83; doi: 10.1016/j.ica.2012.11.023 (c. 19, F.I. 2,7)
39. "The sound of Chemistry: translating infrared wavenumbers into musical notes" N. Garrido, A. Pitto-Barry, J.J. Solevila-Barreda, A. Lupan, L. Comerford Boyes, W.H.C. Martin, N.P.E. Barry, *J. Chem. Educ.*, 2020, *97*, 703-709; doi: 10.1021/acs.jchemed.9b00775 (c. 9, F.I. 2,5)
40. "Six-vertex hydrogen-rich $Cp_2M_2B_4H_8$ dimetallaboranes of the second- and third-row transition metals: effects of skeletal electron count on preferred polyhedra" A.M.V. Branzanic, A. Lupan*, R.B. King, *Organometallics*, 2014, *33*, 6443-6451; doi: 10.1021/om500801e (c. 6, F.I. 2,5)
41. "Binuclear ethylenedithiolate iron carbonyls: a density functitonal theory study" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan*, R.B. King, *Inorg. Chim. Acta*, 2021*, 519,* 120260; doi: 10.1016/j.ica.2021.120260 (c. 4, F.I. 2,7)
42. "Dimetallaboranes with polyhedral surface metal–metal multiple bonds: Deltahedral dirhenaboranes with pentalenedirhenium vertices" A. Lupan, R.B. King, *Organometallics*, 2013, 32, 4002; doi: 10.1021/om400481c (c. 9, F.I. 2,5)
43. "Sulfur and carbon as heteroatoms in ferrathiacarboranes" A.A. Attia, A. Lupan, R.B. King, *Polyhedron*, 2016, *113*, 109-114; doi:10.1016/j.poly.2016.04.027 (F.I. 2,4)
44. "Comparison of hypoelectronic deltahedral ditechnetaboranes having eight to twelve vertices with their rhenium analogues: Examples of polyhedral surface metal–metal multiple bonds" A. Lupan, R.B. King, *Polyhedron*, 2013, *60*, 151; doi: 10.1016/j.poly.2013.04.053 (c. 6, F.I. 2,4)
45. "A phenotypic assay to identify Chikungunya virus inhibitors targeting the nonstructural protein nsP2" M. Lucas-Hourani, A. Lupan, P. Despres, J. Dubois, C. Guillou, F. Tangy, P.O. Vidalain, H. Munier-Lehmann, *J. Biomol. Screen.*, 2013, *18*, 172; doi: 10.1177/1087057112460091 (c. 32, F.I. 2,3)
46. "Metal-metal multiple bonds with “half-bond” components in paramagnetic organometallics of f-block metals" C. Cosar, A.A. Attia, A. Lupan*, R.B. King, *J. Organometal. Chem.*, 2017, *827*, 105-111; doi: 10.1016/j.jorganchem.2016.11.006 (c. 2, F.I. 2,1)
47. "Performance comparison of computational methods for modeling alpha-helical structures" A. Lupan, A. Kun, F. Carrascoza, R. Silaghi-Dumitrescu, *J. Mol. Model.*, 2013, *19*, 193; doi: 10.1007/s00894-012-1531-z (c. 14, F.I. 2,1)
48. "Secondary structure elements in polylactic acid models" I. Irsai, C. Majdik, A. Lupan, R. Silaghi-Dumitrescu, *J. Math. Chem.*, 2012, *50*, 703; doi: 10.1007/s10910-011-9919-z (c. 8, F.I. 1,7)
49. "Weak sulfur-sulfur interactions between chemically-identical atoms" R. Silaghi-Dumitrescu, A. Lupan, *Cent. Eur. J. Chem.*, 2013, *11*, 457; doi: 10.2478/s11532-012-0178-z (c. 14, F.I. 1,46)
50. "Kinetics of reduction of cobalamin by sulfoxylate in aqueous solutions" D.S. Salnikov. I.A. Derevenkov, S.V. Makarov, E.S. Ageeva, A. Lupan, M. Surducan, R. Silaghi-Dumitrescu, *Rev. Roum. Chim.*, 2012, *57*, 353 (c. 20, F.I. 0,4)

27.01.2026