

Alexandru Lupan – listă de publicații

1. "Decarbonylation products of binuclear methylphosphinidene complexes of cyclopentadienyliron carbonyls: triplet and quintet structures are favored energetically over singlet structures with iron-iron multiple bonding" O. Rudenco, A. Lupan*, R. Silaghi-Dumitrescu, R.B. King, *ACS Omega*, **2024**, 9, 12125-12134. doi:10.1021/acsomega.3c10460
2. "A theoretical study of the effect of phosphorus and nitrogen heteroatoms on pentahapto coordination of diazaphospholyl ligands in binuclear ruthenium and iron carbonyl derivatives" T.M. Danescu, R. A. Lupan*, Silaghi-Dumitrescu, R.B. King, *J. Organomet. Chem.*, **2024**, 1004, 122949
3. "Dual spherical-spherical aromaticity in $[M(\eta^2-P_4)_2]^+$ (M = Cu, Ag, Au) and $[P(P_4)_2]^+$. Evaluation of bonding nature and spherical aromatic character of the P_4 aggregates from DFT calculations" C.O. Ulloa, A.A. Attia, A. Lupan, R.B. King, A. Munoz-Castro, *Inorg. Chem. Commun.*, **2024**, 159, 111680; doi: 10.1016/j.inoche.2023.111680
4. "A study of the molecular interactions of hemoglobin with diverse classes of therapeutic agents" C. Zagrean-Tuza, I. Igescu, A. Lupan, R. Silaghi-Dumitrescu, *Inorg. Chim. Acta*, **2024**, 567, 122053 doi: 10.1016/j.ica.2024.122053
5. "A poly(methyl methacrylate)-ibuprofen composite film as anticorrosive coating of Ti-6Al-4 V surface" J.H. Viteri, N. Cotolan, A. Lupan, A.M.V. Branzanic, G.L. Turdean, *J. Solid State Electrochem.*, **2023**, 24, doi: 10.1007/s10008-023-05681-w
6. "Low-energy high-spin binuclear hexamethylbenzene manganese carbonyl structures with partially bonded benzene rings" M. Arpentì, A. Lupan, R.B. King, *J. Organomet. Chem.*, **2023**, 997, 122792; doi: 10.1016/j.jorganchem.2023.122792
7. "Polyhedral ferraboranes with iron carbonyl vertices: carbonyl migration processes in the iron tetracarbonyl derivatives" A.A. Attia, A. Lupan, R.B. King, *J. Phys. Chem. A*, **2023**, 127, 5887-5898; doi: 10.1021/acs.jpca.3c02944
8. "Effect of the coordination environment on the ability of iron to bind/ activate N_2 : A theoretical study with relevance to the nitrogenase mechanism" R. Doukeh, D. Crăciun, A. Lupan, A.M.V. Branzanic, R. Silaghi-Dumitrescu, *Polyhedron*, **2023**, 243, 116571; doi: 10.1016/j.poly.2023.116571
9. "Synthesis, characterisation, and in vitro cytotoxic Activity of dithiocarbamate glycoconjugate half-Sandwich Ruthenium and Osmium Complexes" J.J. Soldevila-Barreda, A. Pettenuzzo, M. Azmanova, L. Rafols, A.A. Attia, A. Lupan, L. Ronconi, N.P. Barry, A. Pitto-Barry, *Helv. Chim. Acta*, **2023**, 106, e202300064, doi: 10.1002/hlca.202300064

10. "Polyhedral dicobaltadithiaboranes and dicobaltdiselenaboranes as examples of bimetallic *nido* structures without bridging hydrogens" A.A. Attia, A. Lupan, R.B. King, *Molecules*, **2023**, 28, 2988; doi: 10.3390/molecules28072988
11. "Versatility of thiourea dioxide as redox agent in globins: case study with myoglobin" O. Rudenco, M. Lehene, A. Lupan, C. Zagrean-Tuza, B. Stoean, A. Gaina-Gardiuta, A.M. Ulici, R. Silaghi-Dumitrescu, *Inorg. Chim. Acta*, **2023**, 551, 121474; doi: 10.1016/j.ica.2023.121474
12. "Aromaticity in P₈ allotropes and (CH)₈ analogues: significance of their 40 valence electrons?" A.A. Attia, A. Lupan, R.B. King, *Phys. Chem. Chem. Phys.*, **2023**, 25, 9364-9372; doi: 10.1039/d3cp00147d
13. "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/acs.inorgchem.2c02936
14. "Combining a weak-field rigid chelating bidentate dicarbene ligand with a strong-field carbonyl ligand in binuclear cyclopentadienyliron carbonyl derivatives" C. Balaiu, A. Lupan, R.B. King, *Polyhedron*, **2022**, 219, 115778; doi: 10.1016/j.poly.2022.115778
15. "Cyclopentadienylmetal group 6 metal carbonyl derivatives with 2-propanoneoximate and related ligands" T.M. Danescu, R. Silaghi-Dumitrescu, A. Lupan, R.B. King, *New J. Chem.*, **2021**, 45, 21092-21099; doi: 10.1039/d1nj04379j
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22. "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
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