PERSONAL INFORMATION

Alexandru Lupan

Str. Arany Janos nr. 11, Cluj-Napoca, 400028, Romania

+40-264-59.38.33 5772

alexandru.lupan@ubbcluj.ro

www.chem.ubbcluj.ro

alexandru.lupan@gmail.com

Sex M | Date of birth 23/05/1978 | Nationality Romanian

POSITION

Associate professor at the Faculty of Chemistry and Chemical Engineering of the Babeș-Bolyai University in Cluj-Napoca, Romania

WORK EXPERIENCE

2017 - 2021 — Lecturer

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Courses and seminars of Structural Chemistry and Molecular medicine and imagistic techniques and research activity in molecular modelling and quantum chemistry

Business or sector public university

2019 - present — Project director PN-III-P2-PED-2293

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Semi-artificial oxygen carriers”

Business or sector public university

2017 - 2019 — Project director PN-III-P4-PCE-0089

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Molecular metal clusters: bridging the gap between small molecules and nanocrystals”

Business or sector public university

2015 - 2017 — Project director PN-II-RU-TE-1197

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Polyhedral metallaboranes: metal clusters stabilized in borane matrices”

Business or sector public university

2014 - 2015 — Project director GTC-334017

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Eight vertex tetrametallaboranes: intermediates between polyhedral boranes and metal clusters”

Business or sector public university

2013 - 2016 — Research assistant

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Redox activation of small molecules at biologic metal centers” (PI prof. dr. Radu Silaghi-Dumitrescu)

Business or sector public university

2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Biomolecule nanomanipulation by atomic force microscopy” (PI acad. prof. dr. Octavian Popescu)

Business or sector public university

2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Biomedical applications of metallic compounds - Metallomics” (PI acad. prof. dr. Ionel Haiduc)

Business or sector public university

2010 - 2013 **Research assistant**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Research activity within the project “Biofunctionalised nanoparticles for developing new imagistic, diagnose, and molecular therapy in biological environments” (PI prof. dr. Simion Aștilean)

Business or sector public university

2006 - 2009 **Postdoctoral researcher**

Chemistry and Biocatalysis unit, Institut Pasteur, Paris, France

- Research activity within the project IdF 06-222_09-1739/2006 “Medicen – chemical library of new chemical entities” (PI CR1 dr. Helene Munier-Lehmann)

Business or sector research institute

2006 - 2017 **Chemist**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Laboratory works in general and inorganic chemistry, molecular modeling and research activity

Business or sector public university

EDUCATION AND TRAINING

2002 - 2006 **Ph. D. in Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Electronic structure calculations of main group cluster compounds

2001 - 2002 **Master in Organometallic and Applied Coordination Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Inorganic chemistry with dissertation in molecular modeling

1997 - 2001 **B. Sc. in Chemistry**

Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University, Cluj-Napoca, Romania

- Chemistry specialisation with dissertation in coordination chemistry

1993 - 1997 **Baccalaureate**

Gheorghe Șincai High School, Cluj-Napoca, Romania

- Chemistry-Biology specialisation

PERSONAL SKILLS

Mother tongue(s): Romanian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C2	C2	C2	C2	C2
French	C2	C2	C2	C2	C2

Levels: A1/2: Basic user - B1/2: Independent user - C1/2 Proficient user
Common European Framework of Reference for Languages

Communication skills
- good communication skills adapted for teaching and mentoring student research activities
- good communication as member of various research teams
- adaptation to multicultural environments and collaboration with other universities

Organisational / managerial skills
- managing research activities as team leader of various research projects

Job-related skills
- good command of quality control processes and acquisitions

Computer skills
- electronic structure calculations, i.e. molecular mechanics, semiempirical, ab initio, post-Hartree Fock, DFT, NBO analysis, TD-DFT, using specialised software such as Gaussian, Gamess, Mopac, Spartan, NWChem.

Other skills
- Experimental and virtual screening techniques, enzymatic analysis and kinetics

Driving licence
- B

ADDITIONAL INFORMATION

ResearcherID: http://www.researcherid.com/rid/A-3142-2012
Presentations: https://www.researchgate.net/profile/Alexandru_Lupan2
Google Scholar: https://scholar.google.com/citations?user=tU6Xp6AAAAAJ&hl=en

Publications - articles

1. "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
2. "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
3. "Isocloso versus closo deltahedra in slightly hypoelectronic supraicosahedral 14-vertex dimetallaboranes with 28 skeletal electrons: relationship to icosahedral dimetallaboranes" S. Jákó, A. Lupan*, A.Z. Kun, R.B. King, New J. Chem., 2020, 44, 16977-16984; doi: 10.1039/d0nj03572f
4. "Enhncement of ion pairing o Sr(II) and Ba(II) salts by a tritopic ion-pair receptor in solution" B. Kutus, J. Zhu, J. Luo, Q.Q. Wang, A. Lupan, A.A. Attia, D.-X. Wang, J. Hunger, ChemPhysChem, 2020, 21, 1957-1965; doi: 10.1002/cphc.202000507
5. "Novel non-spherical deltahedra in tetramolybdaborane structures: Generation of low-energy structures by capping Mo4B4 cubes" A.A. Attia, A. Lupan*, R.B. King, Polyhedron, 2020, 187, 114626; doi: 10.1016/j.poly.2020.114626
6. "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
7. "Nonsphericity in diferratetracarbaboranes having 2n + 2 Wadean skeletal electrons: deviations from closo deltahedral geometries and high-energy kinetically stable isomers" A.A. Attia, A. Lupan*, R.B. King, Phys. Chem. Chem. Phys., 2020, 22, 2437-2448; doi: 10.1039/c9cp04777h
8. "Neutral rhenadicarbaboranes with Re(CO)2(NO) vertices: a theoretical study of building blocks for rhenacarborane-based drug delivery agents" A.A. Attia, A. Lupan*, R. Silaghi-Dumitrescu, R.B. King, Molecules, 2020, 25, 110; doi: 10.3390/molecules25010110
9. "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

10. "The group 9 cyclopentadienylmetal cis Ethylenedithiolates as Metallodithiolene Ligands in Metal Carbonyl Chemistry: Analogies to Benzene Metal Carbonyl Complexes" L.F. Radu, A.A. Attia, R. Silaghi-Dumitrescu, A. Lupan*, R.B. King, New J. Chem., 2019, 43, 12711-12718; doi: 10.1039/C9NJ02478F
11. "Design, synthesis and structure of novel dendritic G-2 melamines comprising piperidine motifs as key linkers and 4-(n-octyloxy)aniline as a peripheral unit" C. Sacalis, C. Morar, P. Lameiras, A. Lupan, R. Silaghi-Dumitrescu, A. Bende, G. Katona, D. Porumb, D. Harakat, E. Gal, M. Darabantu, Tetrahedron, 2019, 75, 130468; doi: 10.1016/j.tet.2019.130468
12. "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
13. "Versatile coordination behaviour of chloro-tetrazine-picolylamine ligand: mixed-valence binuclear Cu(I)/Cu(II) complexes" O. Stetsiuk, S. R. Petrusenko, Lorenzo Sorace, A. Lupan, A. Attia, V. Kokozay, A. El-Ghayoury, N. Avarvari, Dalton Trans., 2019, 48, 11966-11977; doi: 10.1039/C9DT02379H
14. "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.9600289
15. "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
16. "The isocloso capped pentagonal bipyramid versus the closo bisdisphenoid in hypoelectronic eight-vertex metallaboranes having 16 skeletal electron" R.A. Șeptelean, A.A. Attia, A. Lupan*, R.B. King, Int. J. Quant. Chem., 2019, 119, e25880; doi: 10.1002/qua.25880
17. "Calcium complexing behaviour of lactate in neutral to highly alkaline medium" Cs. Dudas, B. Kutus, E. Boszormenyi, G. Peintler, A.A. Attia, A. Lupan, Z. Kele, P. Sipos, I. Palinko, J. Mol. Struct., 2019, 1180, 491-498; doi: 10.1016/j.molstruc.2018.12.020
18. "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
19. "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
20. "Segregation of tetracarbon units in low-energy tetracarbindane structures: major differences from their aluminum and gallium analogues" A.A. Attia, A. Lupan*, R.B. King, Int. J. Quant. Chem., 2019, 119, e25934; doi: 10.1002/qua.25934
21. "The acidity and self-catalyzed lactonization of L-gulonic acid: Thermodynamic, kinetic and computational study" B. Kutus, G. Peintler, A Bucko, Z. Balla, A. Lupan, A.A. Attia, I. Palinko, P. Sipos, Carbohydrate Res., 2018, 467, 14-22; doi: 10.1016/j.carres.2018.07.006
22. "Opening cobaltadicarbaborane deltahedra by external dimethylamino substituents: conversion of icosahedra to isonido 12-vertex polyhedra" A.A. Attia, A. Lupan*, R.B. King, Polyhedron, 2018, 151, 458-464; doi: 10.1016/j.poly.2018.06.003
23. "Binuclear pentalene titanium carbonyls: comparison with related cyclopentadienyltitanium carbonyls" L.F. Radu, A.A. Attia, A. Lupan*, R.B. King, Int. J. Quant. Chem., 2018, 118, e25762; doi: 10.1002/qua.25762
24. "Polyhedral trimetallaboranes of the group 9 metals: isocloso versus capped and uncapped closo deltahedra" A.A. Attia, A. Lupan*, R.B. King, Organometallics, 2018, 37, 1845-1851; doi: 10.1021/acs.organomet.8b00077
25. "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
26. "Group 9 metallatelluraboranes: comparison with their sulfur analogues" A.A. Attia, A. Lupan*, R.B. King, J. Organomet. Chem., 2018, 865, 145-151; doi: 10.1016/j.jorganchem.2018.01.058
27. "Major differences between preferred tetracarbagallane and tetracarbalane structures" A.A. Attia, A. Lupan*, R.B. King, J. Organomet. Chem., 2018, 864, 88-96; doi: 10.1016/j.jorganchem.2018.01.051
28. "Tetracapped tetrahedral ruthenium-sulfur clusters related to iron-sulfur structural units in metalloenzymes" A. Lupan, R. Silaghi-Dumitrescu, R.B. King, Inorg. Chim. Acta, 2018, 475, 193-199; doi:10.1016/j.ica.2017.10.011
29. "Metal-metal bonding in deltahedral dimetallaboranes and trimetallaboranes: a density functional theory study" A.A. Attia, A. Lupan*, R.B. King, Pure Appl. Chem., 2018, 90, 643-652; doi: 10.1515/pac-2017-0906
30. "Aluminum-poor hexacarbalane structures: the transition from localized organoaluminum structures to delocalized polyhedra" A.A. Attia, A. Lupan*, R.B. King, Int. J. Quant. Chem., 2018, 118, e25506; doi: 10.1002/qua.25506
31. "Binuclear pentalene titanium carbonyls involved in the deoxygenation of carbon dioxide" L.F. Radu, A.A. Attia, A. Lupan*, R.B. King, J. Organomet. Chem., 2018, 867, 201-207; doi: 10.1016/j.jorganchem.2017.11.006
32. "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
33. "Computational investigation of spectroscopic parameters in putative secondary structure elements for polylactic acid and comparison with experiment" I. Irsai, A. Lupan, C. Majdik, R. Silaghi-Dumitrescu, Studia Chemia, 2017, 62, 495-513; doi: 10.24193/subbchem.2017.4.42
34. "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
35. "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

36. "Novel non-spherical deltahedra in tritungstaboranes related to the experimentally known Cp*3W3(H)B8H8" A.A. Attia, A. Lupan*, R.B. King, New J. Chem., 2017, 41, 10640-10651; doi: 10.1039/C7NJ01801K
37. "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.2016.11.001
38. "Hexacarbalane structures with 2n+8 skeletal electrons: decorating an aluminum cube with carbon atoms" A.A. Attia, A. Lupan*, R.B. King, Organometallics, 2017, 36, 1019-1026; doi: 10.1021/acs.organomet.7b00001
39. "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
40. "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
41. "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
42. "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
43. "Tetracarbaboranes: nido structures without bridging hydrogens" A.A. Attia, A. Lupan*, R.B. King, Dalton Trans., 2016, 45, 18541-18551; doi: 10.1039/C6DT03507H
44. "Hydrogen migration in hypoelectronic biicosahedral metallaborane structures" A.A. Attia, A. Lupan*, R.B. King, RSC Adv., 2016, 6, 87096-87102; doi: 10.1039/C6RA16304A
45. "Molybdatricarbaboranes as examples of isocloso metallaborane deltahedra with three carbon vertices" A. Lupan*, R.B. King, J. Comput. Chem., 2016, 37, 64-69; doi:10.1002/ jcc.23995
46. "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
47. "Dimetallaborane analogues of the octaboranes of the type Cp2M2B6H10: structural variations with changes in the skeletal electron count" A.M.V. Brânzanic, A. Lupan*, R.B. King, Dalton Trans., 2016, 45, 9354-9362; doi: 10.1039/C6DT00985A
48. "Novel Non-spherical Deltahedra in Trirhenaborane Structures" A.A. Attia, A. Lupan*, R.B. King, New J. Chem., 2016, 40, 7564-7572; doi:10.1039/c6nj01922f
49. "Pairing of carbon atoms in low-energy deltahedral dicarbagallane structures derived from vertex expansion of closo deltahedra" A.A. Attia, A. Lupan*, R.B. King, J. Organometal. Chem., 2016, 819, 173-181; doi: 10.1016/j.jorganchem.2016.06.034
50. "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
51. "Polyhedral cobaltadiselenaboranes: nido structures without bridging hydrogen atoms" A.A. Attia, A. Lupan*, R.B. King, RSC Adv., 2016, 6, 53635-53642; doi: 10.1039/C6RA09821E
52. "Polyhedral dinickelaboranes as analogues of the dicarbaboranes" S. Jákó, A. Lupan*, A.Z. Kun, R.B. King, Polyhedron, 2016, 110, 31-36; doi: 10.1016/j.poly.2016.02.016
53. "Contrasting behavior of the group 15 elements (P, As, Sb, Bi) as heteroatoms in icosahedral cobaltaboranes: effect of phosphorus atom basicity " A.A. Attia, A. Lupan*, R.B. King, Rev. Roum. Chim, 2016, 61, 247-250; WOS:000385693200005
54. "The effect of electron-rich heteroatoms in metallaborane clusters" A. Lupan*, A.A. Attia, R.B. King, Studia Chemia, 2016, 26(3), 91-100; WOS: 000393577300010
55. "Computational Study on the Effect of Axial Ligation Upon the Electronic Structure of Copper (II) Porphyrinate (CuTPPs = [5,10,15,20-tetrakis(N-methylpyridyl-4)porhinato] copper (II) tetratosylate)) - Electronic Structure with Different Axial Ligands" R.-V. Tolan, A. Lupan*, R. Silaghi-Dumitrescu, J. Chem. Soc. Pak., 2016, 38, 405-414; WOS:000381933700005
56. "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
57. "Cyclopentadienylironphosphacarboranes: fragility of polyhedral edges in the 11-vertex system" A.A. Attia, A. Lupan*, R.B. King, RSC Adv., 2016, 6, 1122-1128; doi: 10.1039/10.1039/C5RA17070B
58. "Dimetallaborane analogues of pentaborane" A.M.V. Branzanic, A. Lupan*, R.B. King, Dalton Trans., 2015, 44, 7355-7363; doi: 10.1039/C5DT00143A
59. "The presence of cobaltdibismuth triangular faces in the lowest energy deltahedral cobaltadibismaborane polyhedra: Major differences from their cobaltadiphosphaborane analogues" A.A. Attia, A. Lupan*, R.B. King, J. Organometal. Chem., 2015, 798, 252-256; doi:10.1016/j.jorganchem.2015.04.010
60. "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
61. "The Wade-Mingos rules in seven-vertex dimetallaborane chemistry: hydrogen-rich Cp2M2B5H9 systems of the second and third row transition metals" A.M.V. Branzanic, A. Lupan*, R.B. King, J. Organometal. Chem., 2015, 792, 74-80; doi: 10.1016/ j.jorganchem.2015.02.030
62. "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
63. "Phosphorus as a heteroatom in metallaborane structures: cyclopentadienylcobalt diphosphaboranes" A.A. Attia, A. Lupan*, R.B. King, Polyhedron, 2015, 85, 933-940; doi:10.1016/j.poly.2014.10.005
64. "Designing a non-icosahedral twelve-vertex deltahedral metallatricarbaborane with a degree 7 metal vertex" A. Lupan*, R.B. King, Inorg. Chem. Commun., 2015, 51, 40-41; doi: 10.1016/j.inoche.2014.11.003
65. "Cyclopentadienylcobalt azaboranes violating the Wade-Mingos rules: a degree 3 vertex for the nitrogen atom" A.A. Attia, A. Lupan*, R.B. King, RSC Adv., 2015, 5, 56885-56890; doi: 10.1039/C5RA09849A
66. "Six-vertex hydrogen-rich Cp2M2B4H8 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

67. "Sulfur as a heteroatom in metallaborane structures: cyclopentadienylcobalt thiaboranes" A. Lupan*, R.B. King, Polyhedron, 2014, 78, 130-134; doi: 10.1016/j.poly.2014.04.041
68. "The buildup of eight-vertex tetrametallaborane clusters: bisdisphenoidal versus tetracapped tetrahedral structures" A. Lupan*, R.B. King, Eur. J. Inorg. Chem., 2014, 22, 3614-3618; doi: 10.1002/ejic.201402363
69. "Deltahedral ferratricarbaboranes: analogues of ferrocene" A. Lupan*, R.B. King, Dalton Trans., 2014, 43, 4993-5000; doi: 10.1039/C3DT52381K
70. "Structural and electronic isomerism in Fe,S centers" A. Lupan*, A. Attia, R. Silaghi-Dumitrescu, S.V. Makarov, A.F. Vanin, J. Biol. Inorg. Chem., 2014, 19, S279; WOS:000332835300220
71. "Flattened deltahedral structures and bridging hydrogen atoms in hypoelectronic dimolybdaboranes and ditungstaboranes" A. Lupan*, R.B. King, J. Organomet. Chem., 2014, 754, 94-103; doi: 10.1016/j.jorganchem.2013.12.045
72. "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
73. "Pentalene as a ligand in hypoelectronic diruthenaboranes and diosmaboranes with surface metal-metal double bonding" A. Lupan*, R.B. King, Polyhedron, 2014, 71, 133-141; doi: 10.1016/j.poly.2014.01.010
74. "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
75. "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
76. "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
77. "Hypoelectronic diruthenaboranes and diosmaboranes having eight to twelve vertices: capped isocloso and bicapped closo structures" A. Lupan, R.B. King, New J. Chem., 2013, 37, 2528; doi: 10.1039/C3NJ00460K
78. "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
79. "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
80. "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
81. "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
82. "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
83. "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
84. "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
85. "Phosphinoarylthiolato molybdenum and iron complexes M{(SC6H4-2-PPh2)-kappa S-2,P}(2) (CO)(2) (M = Mo, Fe): Analogous composition - Different structure" A.M. Valean, S. Gomez-Ruiz, A. Lupan, R. Silaghi-Dumitrescu, L. Silaghi-Dumitrescu, E. Hey-Hawkins, Inorg. Chim. Acta, 2013, 394, 289; doi: 10.1016/j.ica.2012.05.041
86. "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
87. "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
88. "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
89. "Kinetic versus thermodynamic isomers of the deltahedral dicobaltadicarbaboranes having nine to 12 vertices" A. Lupan, R.B. King, Polyhedron, 2012, 33, 319; doi: 10.1016/ j.poly.2011.11.042
90. "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
91. "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
92. "Can geometrical distortions make a laccase change color from blue to yellow?" A. Lupan*, C. Matyas, A. Mot, R. Silaghi-Dumitrescu, Stud. Univ. Babes-Bolyai Chem., 2011, 56, 231.
93. "Interactions between proteins and platinum-containing anti-cancer drugs" C. Bischin, V. Taciuc, A. Lupan, R. Silaghi-Dumitrescu, Minirev. Med. Chem., 2011, 11, 214; doi: 10.2174/138955711795049844
94. "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
95. "PM6 modeling of alpha-helical polypeptide structures" A. Kun, A. Lupan, R. Silaghi-Dumitrescu, Stud. Univ. Babes-Bolyai Chem., 2010, 55, 265.
96. "New low symmetry low energy structures of 11-atom bare germanium clusters: A density functional theory study" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, Chem. Phys., 2006, 327, 344; doi: 10.1016/j.chemphys.2006.05.006
97. "A quantum chemical conformational analysis of p-tert-butyl/pentyl/octyl-calix[8]arenes" A. Lupan, A. Saponar, I. Silaghi-Dumitrescu, A. Kun, L. Silaghi-Dumitrescu, E.J. Popovici, Stud. Univ. Babes-Bolyai Chem., 2006, 51, 27.

98. "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
99. "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
100. "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
101. "Germanium cluster polyhedra: A density functional theory study" I. Silaghi-Dumitrescu, A. Kun, A. Lupan, R.B. King, Adv. Comput. Met. Sci. Eng., 2005, 4, 804; WOS:000238054400199
102. "The shapes of hypoelectronic six-vertex anionic bare boron clusters: Effects of the countercations" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, A. Kun, Main Group Chem., 2005, 4, 291; doi: 10.1080/10241220600798435

Book chapters

1. "Beyond the Wade-Mingos rules: deviations from sphericality in metallaborane structures" A. Lupan, A.A. Attia, Sz. Jako, A.Z. Kun, R.B. King, in "Structure and Bonding" (book series) edited by D.M.P. Mingos, 2021, https://link.springer.com/chapter/10.1007/430_2021_83
2. "Metal-metal multiple bonding in dimetallaboranes" A. Lupan, R.B. King, chapter in the book "Handbook of boron chemistry in organometallics, catalysis, materials and medicine", edited by N. Hosmane, R. Eagling; World Scientific, 2018, ISBN 978-1-78634-441-0 http://www.worldscientific.com/worldscibooks/10.1142/q0130
3. "Computational studies of metallaboranes and metallacarboranes" A. Lupan*, R.B. King, chapter in the book "Boron - the fifth element", edited by D. Hnyk, M.L. McKee; Springer, 2015, p. 49-95, ISBN 978-3-319-22282-0 http://www.springer.com/gp/book/9783319222813
4. "Computational modelling metal-protein interactions: cisplatin" A. Lupan*, A. Kun, R. Silaghi-Dumitrescu, Metal Elem. Environ. Med. Biol., 2010, 199.

Patents

1. "Identifying modulators of virulence of Alphavirus by comparing the activity of the first reporter gene to a control mammalian cell not expressing the non-structural protein 2 (nsP2) coding sequence and comprising the first reporter gene" Y. Jacob, M. Lucas-Hourani, F. Tangy, P.O. Viadalain, A. Lupan, H. Munier-Lehmann, 2009 EU Patent EP2065476-A1 WO2009068998-A1 https://patents.google.com/patent/WO2009068998A1
2. "Identifying agent that induces interferon stimulated response element, where agent is useful to treat e.g. cancer and viral infection, comprises contacting test agent with cell and detecting agent that results in activation of reporter gene" Y. Jacob, M. Lucas-Hourani, A. Lupan, H. Munier-Lehmann, F. Tangy, P.O. Viadalain, 2011 US Patent US2011159480-A1 WO2011080686-A1 https://patents.google.com/patent/WO2011080686A1

Conferences

1. "Beyond the Wade-Mingos rules: deviations from sphericality in metallaborane structures" A. Lupan, A.A. Attia, Sz. Jako, A.Z. Kun, R.B. King, Zilele Academice Clujene 2021. 21 - 22 October 2021, Cluj-Napoca, Romania (oral presentation, online conference)
2. "Paramagnetism and metal-metal bonding in metallaboranes" A. Lupan, Sz. Jako, A.Z. Kun, R.B. King; EuroBoron 8 – 8th European Conference on Boron Chemistry, 24 - 27 iunie 2019, Montpellier, France (oral presentation)
3. "Unusual polyhedral in organoaluminum carbon clusters: a theoretical view" A. Lupan, A.A. Attia, R.B. King; ICOMC 2018 – 28th International Conference on Organometallic Chemistry, 15 - 20 iulie 2018, Florence, Italy (invited lecture)
4. "Unusual polyhedral in group 13 metal-carbon clusters: a theoretical study" A. Lupan, A.A. Attia, R.B. King; ICCC 2018 – 43rd International Conference on Coordination Chemistry, 30 iulie - 4 august 2018, Sendai, Japonia (oral presentation)
5. "Theoretical studies on polyhedral metallaboranes containing transition metals" Sz. Jako, A. Lupan, A.Z. Kun, R.B. King; YRICCCE II – International Conference on Chemistry and Chemical Enginnering, 3 - 5 mai 2018, Budapesta, Ungaria (oral presentation)
6. "Polyhedral metallaboranes with group fifteen heteroatoms" A. Lupan, A.A. Attia, R.B. King; IMEBORON XVI - International Meeting on Boron Chemistry, 9 - 13 iulie 2017, Hong Kong, China (oral presentation)
7. "Embedding metal atoms in icosahedral structures: biicosahedral metallaboranes as three-dimensional analogues of naphtalene" A. Lupan, A.A. Attia, R.B. King; WATOC 2017 – 11th Triennial Congress of the World Association of Theoretical and Computational Chemists, 27 august - 1 septembrie 2017, Munchen, Germania (poster presentation)
8. "Polyhedral metallaboranes with group 15 heteroatoms" A. Lupan, A.A. Attia, R.B. King; ICOMC - International Conference on Organometallic Chemistry, 17 - 22, iulie 2016, Melbourne, Australia (oral presentation)
9. "Mixed aluminum-carbon clusters in organoaluminum chemistry" A. Lupan, A.A. Attia, R.B. King; ClusPom Conference (Clusters and Polyoxometalates), 29 iunie - 2 iulie, Rennes, Franta 2016 (oral presentation)
10. "Group 15 elements as vertex atoms in metallaboranes" A. Lupan, A.A. Attia, R.B. King; ICCC - International Conference on Coordination Chemistry, 3-8 iulie 2016, Brest, Franta (poster presentation)
11. "Metallaboranes containing main group heteroatoms" A. Lupan, A.A. Attia, R.B. King; YYRICCCE I - Young Researchers' International Conference on Chemistry and Chemical Engineering, 12 - 15 May 2016, Cluj-Napoca, Romania (oral presentation)
12. "Tetracapped tetrahedral ruthenium-sulfur clusters as cubanoid low-spin models for iron-sulfur structural units in metalloenzymes" A. Lupan, R. Silaghi-Dumitrescu, R.B. King, ICBIC-17 - The 17th International Conference on Biological Inorganic Chemistry, 20 - 24 iulie 2015, Beijing, China (poster presentation)
13. "From closo to isocloso deltahedra and beyond in metallaborane chemistry" A. Lupan, R.B. King; IMEBORON XV - International meeting on boron chemistry, 24-28 august 2014, Praga, Cehia, (oral presentation)
14. "DFT study of metallaborane polyhedra" A. Lupan, R.B. King; 7th edition of Molecular Modeling in Chemistry and Biochemistry, 13 - 15 november 2014, Cluj-Napoca, Romania (oral presentation)
15. "Structural and electronic isomerism in Fe,S centers" A. Lupan, A.A. Attia, R. Silaghi-Dumitrescu, R.B. King, ICBIC-16 - The 16th International Conference on Biological Inorganic Chemistry, 22 - 26 iulie 2013, Grenoble, Franta (poster presentation)
16. "Density functional theory study of the deltahedral dicobaltadicarbaboranes having 9 to 12 vertices" A. Lupan, R.B. King, 4th EuCheMS Chemistry Congress, 26-30 august 2012, Praga, Cehia (poster presentation)

17. "Siroheme-containing sulfite reductase: density functional theory investigations of the mechanism" A. Lupan, M. Surducan, D. Lup, S. Makarov, R. Silaghi-Dumitrescu; Eurobic-11 - The 11th European Biological Inorganic Chemistry Congress, 12-16 septembrie 2012, Granada, Spania (poster presentation)
18. "Metal-metal multiple surface bonding in polyhedral metallaborane clusters" A. Lupan, R.B. King; WATOC-10 - The tenth triennial congress of the World Association of Theoretical and Computational Chemists, 5-10 octombrie 2014, Santiago de Chile, Chile, (poster presentation)
19. "Performance of computational methods for modeling alpha helical structures" A. Lupan, A.Z. Kun, R. Silaghi-Dumitrescu WATOC-9 - The nineth triennial congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spania, 17 - 22 iulie 2011 (poster presentation)
20. "Ab initio modeling of secondary structure elements in proteins. Interactions with cisplatin and related compounds" A. Lupan*, A.-Z. Kun, R. Silaghi-Dumitrescu, The XXXI-st Romanian Chemistry Conference, Ramnicu-Valcea, Romania, 6-8 octombrie 2010 (poster presentation)
21. "Ab initio modeling of secondary structure elements in proteins" A. Lupan, R. Silaghi-Dumitrescu, 7th Interneational Conference of the Chemical Societies of the Chemical Societies of the South-Eastern European Countries, 15-17 septembrie 2010, Bucuresti, Romania (poster presentation)
22. "Localized versus delocalized surface electrons in borane/germanium clusters" A. Lupan, R.B. King, I. Silaghi-Dumitrescu, TopMol Conference, Cluj-Napoca, Romania, 25-30 septembrie 2006 (poster presentation)
23. "Low symmetry low energy structures of 11-atom bare germanium clusters: a density functional theory study" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, Third Humboldt Conference on Computational Chemistry, Varna, Bulgaria, 24-28 iunie 2006 (poster presentation)
24. "Distortions from octahedral symmetry in hypoelectronic six-vertex polyhedral boron clusters as studied by ab initio methods: effects of alkali-metals countercations" R.B. King, A. Lupan, A.Z. Kun, I. Silaghi-Dumitrescu, International Conference 'Molecular Modeling' in Chemistry and Biochemistry, Cluj-Napoca, Romania, 21-23 aprilie 2005 (oral presentation)
25. "Distorsii de la simetria octaedrica in clusteri hipoelectronici poliedrali cu sase varfuri ai borului studiate prin metode ab initio" A. Lupan, R.B. King, A.Z. Kun, I. Silaghi-Dumitrescu, A XXVIII-a Conferinta Nationala de Chimie, Calimanesti-Caciulata, Romania, 6-8 octombrie 2004 (poster presentation)

Memberships Romanian Chemical Society