INFORMAŢII PERSONALE

Alexandru Lupan



Str. Arany Janos nr. 11, Cluj-Napoca, 400028, România
+40-264.59.38.33 5772
alexandru.lupan@ubbcluj.ro
www.chem.ubbcluj.ro
alexandru.lupan@gmail.com

Sexul M | Data naşterii 1978 | Naţionalitatea Română

POZIŢIA
2021- prezent

Conferențiar universitar abilitat la Facultatea de Chimie și Inginerie Chimică a Universității Babeș-Bolyai din Cluj-Napoca, România

EXPERIENŢA PROFESIONALĂ

2017 - 2021

Lector universitar

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Cursuri și seminarii de Structură Chimică și Medicină Moleculară și Tehnici de Imagistică și activitate de cercetare în modelare moleculară și chimie cuantică

Tipul sau sectorul de activitate universitate publică

2020 - 2022

Director proiect PN-III-P2-PED-2293

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului “Transportori semiartificiali de oxigen”

Tipul sau sectorul de activitate universitate publică

2017 - 2019

Director proiect PN-III-P4-PCE-0089

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului “Clusteri metalici moleculari: o punte între molecule mici și nanocristale”

Tipul sau sectorul de activitate universitate publică

2015 - 2017

Director proiect PN-II-RU-TE-1197

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului “Metalaborani poliedrali: clusteri metalici stabilizați în matrici boranice”

Tipul sau sectorul de activitate universitate publică

2014 - 2015

Director proiect GTC-334017

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului “Tetrametalaborani cu opt vârfuri: intermediari între borani poliedrali și clusteri metalici”

Tipul sau sectorul de activitate universitate publică

2013 - 2013

Asistent cercetare

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului “Activarea redox a moleculelor mici la centri metalici biologici” (director proiect prof. dr. Radu Silaghi-Dumitrescu)

Tipul sau sectorul de activitate universitate publică

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2010 - 2013 **Asistent cercetare**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului "Nanomanipularea biomoleculelor prin microscopie de forță atomică" (director proiect acad. prof. dr. Octavian Popescu)

Tipul sau sectorul de activitate universitate publică

2010 - 2013 **Asistent cercetare**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului "Aplicații biomedicale ale compușilor metalici - Metallomics" (director proiect acad. prof. dr. Ionel Haiduc)

Tipul sau sectorul de activitate universitate publică

2010 - 2013 **Asistent cercetare**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Activitate de cercetare în cadrul proiectului "Nanoparticule biofuncționalizate pentru dezvoltarea de noi medii pentru imagistică, diagnoză și terapie moleculară" (director proiect prof. dr. Simion Aștilean)

Tipul sau sectorul de activitate universitate publică

2010 - 2013 **Cercetător postdoctoral**

Unitatea de Chimie și Biocataliză, Institutul Pasteur, Paris, Franța

- Activitate de cercetare în cadrul proiectului IdF 06-222_09-1739/2006 "Medicen – librărie chimică de noi entități chimice" (director proiect CR1 dr. Helene Munier-Lehmann)

Tipul sau sectorul de activitate universitate publică

2006 - 2017 **Chimist**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Lucrări de laborator de chimie generală, chimie anorganică, modelare moleculară și activ. cercetare

Tipul sau sectorul de activitate universitate publică

EDUCAŢIE ŞI FORMARE

2002 - 2006 **Doctorat în Chimie**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Investigarea unor clusteri metalici prin calcule de structură electronică

2001 - 2002 **Masterat în Chimie Organometalică și Coordinativă Aplicată**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Chimie anorganică și disertație în domeniul modelării moleculare

1997 - 2001 **Licență în Chimie**

Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România

- Specializarea Chimie și licență în chimie coordinativă

1993 - 1997 **Bacalaureat**

Liceul Gheorghe Șincai, Cluj-Napoca, România

- Specializarea Chimie-Biologie

COMPETENTE PERSONALE

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Limba(i) maternă(e) Română

Alte limbi străine cunoscute

	INTELEGERE		VORBIRE		SCRIERE
	Ascultare	Citire	Participare la conversaţie	Discurs oral	
Engleză	C2	C2	C2	C2	C2
Franceză	C2	C2	C2	C2	C2

Niveluri: A1/2: Utilizator elementar - B1/2: Utilizator independent - C1/2: Utilizator experimentat
Cadrul european comun de referinţă pentru limbi străine

Competenţe de comunicare
- bune competenţe de comunicare adaptate predării și metoratului activităților de cercetare
- bune competențe de comunicare ca și membru al unor echipe de cercatre
- adaptarea la medii multiculturale și colaborarea cu alte universități

Competenţe organizaţionale/manageriale
- activitate de management de cercetare ca și director al unor diverse proiecte

Competenţe dobândite la locul de muncă
- o bună cunoaştere a procedurilor administrative

Competenţe informatice
- calcule de structură electronică, mecanică moleculară, semiempirice, ab initio, post-Hartree Fock DFT, analiză NBO, TD-DFT, folosind programe specializate precum Gaussian, Gamess, Mopac, Spartan, NWChem.

Alte competenţe
- tehnici de screening experimental și virtual, analiză și cinetică enzimatică

Permis de conducere
- B

INFORMATII SUPLIMENTARE

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

Publicații - articole

1. "Low-energy high-spin binuclear hexamethylbenzene manganese carbonyl structures with partially bonded benzene rings" M. Arpenti, A. Lupan*, R.B. King, J. Organomet. Chem., 2023, 997, 122792; doi: 10.1016/j.jorganchem.2023.122792
2. "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
3. "Effect of the coordination environment on the ability of iron to bind/ activate N2: 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
4. "Synthesis, characterisation, and in vitro cytotoxic Activity of dithiocarbamato 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
5. "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
6. "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
7. "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
8. "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
9. "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
10. "Cyclopentadienylmetal group 6 metal carbonyl derivatives with 2-propanoneoximato 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
11. "Peroxo-transition metals systems: examples of redox isomerism in palladium structures" I.A. Suciu, R. A. Lupan, Silaghi-Dumitrescu, Rev. Roum. Chim, 2021, 66, 819-828; doi: 10.33224/rrch.2021.66.10-11.05
12. "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
13. "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
14. "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
15. "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
16. "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
17. "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
18. "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
19. "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
20. "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

21. "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
22. "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
23. "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
24. "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
25. "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
26. "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
27. "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
28. "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
29. "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
30. "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
31. "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
32. "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
33. "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
34. "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
35. "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
36. "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
37. "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
38. "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
39. "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
40. "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
41. "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
42. "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
43. "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
44. "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
45. "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
46. "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

47. "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
48. "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
49. "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
50. "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
51. "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
52. "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
53. "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
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55. "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
56. "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
57. "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
58. "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
59. "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
60. "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
61. "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
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Capitole de carte

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Conferințe

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, 17th International Meeting on Boron Chemistry IMEBORON-17, 9 - 13 July 2023, Rennes, France (invited lecture)
2. "Unusual non-spherical deltahedra in metallaborane structures" A. Lupan, A.A. Attia, Sz. Jako, A.Z. Kun, R.B. King, 18th Central European Symposium on Theoretical Chemistry, 7 - 10 September 2022, Balatonszarszo, Hungary (invited lecture)
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4. "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)
5. "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)
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21. "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)
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Alte mențiuni

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