

## INFORMAȚII PERSONALE



## Alexandru Lupan

- 📍 Str. Arany Janos nr. 11, Cluj-Napoca, 400028, România
- ☎ +40-264.59.38.33 📠 5772
- ✉ [alexandru.lupan@ubbcluj.ro](mailto:alexandru.lupan@ubbcluj.ro)
- 🌐 [www.chem.ubbcluj.ro](http://www.chem.ubbcluj.ro)
- 💬 [alexandru.lupan@gmail.com](mailto:alexandru.lupan@gmail.com)

Sexul M | Data nașterii 23/05/1978 | Naționalitatea Română

POZIȚIA  
2021- prezent

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

## EXPERIENȚA 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

2019 - 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 semiaficiali 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

- 2010 - 2013 **Asistent cercetare**  
Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai, Cluj-Napoca, România
- Activitate de cercetare în cadrul proiectului “Nanomanipularea biomoleculilor 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

## EDUCAȚIE ȘI FORMARE

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- 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 conversație	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 referință pentru limbi străine

Competențe de comunicare

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

Competențe organizaționale/manageriale

- activitate de management de cercetare ca și director al unor diverse proiecte

Competențe dobândite la locul de muncă

- o bună cunoaștere a procedurilor administrative

Competențe 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 competențe

- 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](https://www.researchgate.net/profile/Alexandru_Lupan2)  
 Google Scholar <https://scholar.google.com/citations?user=tU6Xp6AAAAAJ&hl=en>

## Publicații - articole

- "Low-energy high-spin binuclear hexamethylbenzene manganese carbonyl structures with partially bonded benzene rings" M. Arpent, A. Lupan\*, R.B. King, J. Organomet. Chem., 2023, 997, 122792; doi: 10.1016/j.jorganchem.2023.122792
- "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
- "Effect of the coordination environment on the ability of iron to bind/ activate N<sub>2</sub>: 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
- "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
- "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
- "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
- "Aromaticity in P<sub>8</sub> allotropes and (CH)<sub>8</sub> 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
- "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
- "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
- "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
- "Peroxo-transition metals systems: examples of redox isomerism in palladium structures" I.A. Suci, R. A. Lupan, Silaghi-Dumitrescu, Rev. Roum. Chim., 2021, 66, 819-828; doi: 10.33224/rch.2021.66.10-11.05
- "Binuclear ethylenedithiolate iron carbonyls: a density functional 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
- "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
- "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
- "Enhancement of ion pairing of 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
- "Novel non-spherical deltahedra in tetramolybdaborane structures: Generation of low-energy structures by capping Mo<sub>4</sub>B<sub>4</sub> cubes" A.A. Attia, A. Lupan\*, R.B. King, Polyhedron, 2020, 187, 114626; doi: 10.1016/j.poly.2020.114626
- "The sound of Chemistry: translating infrared wavenumbers into musical notes" N. Garrido, A. Pitto-Barry, J.J. Soldevila-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
- "Nonsphericity in diferratetracarboranes 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
- "Neutral rhenadithiaboranes with Re(CO)<sub>2</sub>(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
- "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 Metallothiolene 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. Helynyck, 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. Şeptelean, 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 dichromadycarbaborane structures: the nature of Stone's icosahedral dichromadycarbaborane" 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 tetracarbendane 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 cobaltadycarbaborane 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 tetracarbogallane and tetracarbaborane 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 hexacarbaborane 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 Chimica*, 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 metallacarbaboranes: the polyhedral chromadycarbaborane 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. "Hexacarbale 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
54. "Tetracarboranes: nido structures without bridging hydrogens" A.A. Attia, A. Lupan\*, R.B. King, *Dalton Trans.*, 2016, 45, 18541-18551; doi: 10.1039/C6DT03507H
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 dicarbaborane 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 ferrathiocarboranes" A.A. Attia, A. Lupan\*, R.B. King, *Polyhedron*, 2016, 113, 109-114; doi:10.1016/j.poly.2016.04.027
62. "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
63. "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
64. "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
65. "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
66. "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)porphinato] 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
67. "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
68. "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
69. "Dimetallaborane analogues of pentaborane" A.M.V. Branzanic, A. Lupan\*, R.B. King, *Dalton Trans.*, 2015, 44, 7355-7363; doi: 10.1039/C5DT00143A
70. "The presence of cobaltdibismuth triangular faces in the lowest energy deltahedral cobaltdibismaborane polyhedra: Major differences from their cobaltdiphosphaborane analogues" A.A. Attia, A. Lupan\*, R.B. King, *J. Organometal. Chem.*, 2015, 798, 252-256; doi:10.1016/j.jorganchem.2015.04.010
71. "On the roles of alanine and serine in the  $\beta$ -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
72. "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
73. "Nonspherical deltahedra in low-energy dicarbale structures testing the Wade-Mingos rules: the regular icosahedron is not favored for the 12-vertex dicarbale" A.A. Attia, A. Lupan\*, R.B. King, *Inorg. Chem.*, 2015, 54, 11377-11384; doi:10.1021/acs.inorgchem.5b02014
74. "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
75. "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
76. "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
77. "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

78. "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
79. "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
80. "Deltahedral ferratricarbaboranes: analogues of ferrocene" A. Lupan\*, R.B. King, *Dalton Trans.*, 2014, 43, 4993-5000; doi: 10.1039/C3DT52381K
81. "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
82. "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
83. "Microwave assisted synthesis, photophysical and redox properties of (phenothiazinyl) vinyl-pyridinium dyes" L. Gaină, I. Torje, E. Gal, A. Lupan, C. Bischin, R. Silaghi-Dumitrescu, G. Damian, P. Lonneck, C. Cristea, L. Silaghi-Dumitrescu, *Dyes Pigm.*, 2014, 102, 315-325; doi: 10.1016/j.dyepig.2013.10.044
84. "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
85. "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
86. "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
87. "Dimetallaboranes with polyhedral surface metal-metal multiple bonds: Deltahedral diruthenaboranes with pentalenedirhenium vertices" A. Lupan, R.B. King, *Organometallics*, 2013, 32, 4002; doi: 10.1021/om400481c
88. "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
89. "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
90. "Comparison of hypoelectronic deltahedral ditetranaboranes 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
91. "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
92. "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
93. "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
94. "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
95. "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
96. "Phosphinoaryliothiolato molybdenum and iron complexes  $M\{(SC_6H_4-2-PPH_2)\text{-}kappa\text{-}S-2,P\}_2(CO)_2$  ( $M = Mo, Fe$ ): 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
97. "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
98. "Hypoelectronic diruthenaboranes 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
99. "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
100. "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
101. "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
102. "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
103. "Can geometrical distortions make a laccase change color from blue to yellow?" A. Lupan\*, C. Matyas, A. Mot, R. Silaghi-Dumitrescu, *Stud. Univ. Babeş-Bolyai Chem.*, 2011, 56, 231.
104. "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
105. "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
106. "PM6 modeling of alpha-helical polypeptide structures" A. Kun, A. Lupan, R. Silaghi-Dumitrescu, *Stud. Univ. Babeş-Bolyai Chem.*, 2010, 55, 265.
107. "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
108. "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. Babeş-Bolyai Chem.*, 2006, 51, 27.

109. "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
110. "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
111. "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
112. "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
113. "The shapes of hypoelectronic six-vertex anionic bare boron clusters: Effects of the counteranions" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, A. Kun, *Main Group Chem.*, 2005, 4, 291; doi: 10.1080/10241220600798435

#### Capitole de carte

1. "Beyond the Wade-Mingos rules: deviations from sphericity 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](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/g0130>
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, in "Metal Elem. Environ. Med. Biol.", 2010, 199-204, ISSN 1583-4204.

#### Patente

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. Viadalaín, 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. Viadalaín, 2011 US Patent US2011159480-A1 WO2011080686-A1 <https://patents.google.com/patent/WO2011080686A1>

#### Conferințe

1. "Beyond the Wade-Mingos rules: deviations from sphericity 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)
3. "Beyond the Wade-Mingos rules: deviations from sphericity 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)
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)
6. "Unusual polyhedral in group 13 metal-carbon clusters: a theoretical study" A. Lupan, A.A. Attia, R.B. King; ICCS 2018 – 43rd International Conference on Coordination Chemistry, 30 iulie - 4 august 2018, Sendai, Japonia (oral presentation)
7. "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 Engineering, 3 - 5 mai 2018, Budapesta, Ungaria (oral presentation)
8. "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)
9. "Embedding metal atoms in icosahedral structures: biicosahedral metallaboranes as three-dimensional analogues of naphthalene" 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)
10. "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)
11. "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)
12. "Group 15 elements as vertex atoms in metallaboranes" A. Lupan, A.A. Attia, R.B. King; ICCS - International Conference on Coordination Chemistry, 3-8 iulie 2016, Brest, Franta (poster presentation)
13. "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)
14. "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)
15. "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)
16. "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)



17. "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)
18. "Density functional theory study of the deltahedral dicobaltadecaboranes having 9 to 12 vertices" A. Lupan, R.B. King, 4th EuCheMS Chemistry Congress, 26-30 august 2012, Praga, Cehia (poster presentation)
19. "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)
20. "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)
21. "Performance of computational methods for modeling alpha helical structures" A. Lupan, A.Z. Kun, R. Silaghi-Dumitrescu WATOC-9 - The ninth triennial congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spania, 17 - 22 iulie 2011 (poster presentation)
22. "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)
23. "Ab initio modeling of secondary structure elements in proteins" A. Lupan, R. Silaghi-Dumitrescu, 7th Intemeational Conference of the Chemical Societies of the Chemical Societies of the South-Eastern European Countries, 15-17 septembrie 2010, Bucuresti, Romania (poster presentation)
24. "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)
25. "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)
26. "Distortions from octahedral symmetry in hypoelectronic six-vertex polyhedral boron clusters as studied by ab initio methods: effects of alkali-metals counteranions" 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)
27. "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)

## Memberu în asociații

Societatea Română de Chimie