



Curriculum vitae Europass

Personal information

Surname(s) / First name(s) **Lupan Alexandru**
Address **Str. Arany Janos, Nr. 11, Cluj-Napoca, Cluj**
E-mail **alupan@chem.ubbcluj.ro**
Nationality **Romanian**
Date of birth **23.05.1978**

Work experience

Dates **2006-present**
Occupation or position held **Chemist**
Name of employer **Facultatea de Chimie și Inginerie Chimică, Universitatea Babeș-Bolyai**
Principal subjects/occupational skills covered **laboratory work in General Chemistry, research in inorganic and bioinorganic chemistry**

Dates **2007-2010**
Occupation or position held **Postdoctoral researcher**
Name of employer **Institut Pasteur, Paris, France**
Principal subjects/occupational skills covered **Research on the biological activity of chemical compounds**

Education and training

Dates **2002 - 2006**
Title of qualification awarded **PhD in Chemistry**
Name and type of organisation **Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University**

Dates **2001 – 2002**
Title of qualification awarded **Master of Science in Applied Organometallic and Coordination Chemistry**
Name and type of organisation **Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University**

Dates **1997- 2001**
Title of qualification awarded **Bachelor's degree in Chemistry**
Name and type of organisation **Faculty of Chemistry and Chemical Engineering, Babeș-Bolyai University**

Personal skills and competences**Other languages**

English

French

Understanding				Speaking				Writing	
Listening		Reading		Spoken interaction		Spoken production			
C2	advanced	C2	advanced	C2	advanced	C2	advanced	C2	advanced
C2	advanced	C2	advanced	C1	advanced	C1	advanced	C1	advanced

(*) Common European Framework of Reference for Languages

Technical skills and competences

use of specialized Chemistry software (HyperChem, GAMESS, Gaussian, Mopac, Spartan, Flexx, etc.)

ResearcherID<http://www.researcherid.com/rid/A-3142-2012>**Publications**

1. "Dimetallaborane analogues of pentaborane" A.M.V. Branzanic, A. Lupan, R.B. King, *Dalton Trans.*, 2015, *in press*, doi: 10.1039/C5DT00143A
2. "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, *in press*, doi: 10.1016/j.jorganchem.2015.02.030
3. "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
4. "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
5. "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
6. "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
7. "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
8. "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
9. "Deltahedral ferratricarbaboranes: analogues of ferrocene" A. Lupan, R.B. King, *Dalton Trans.*, 2014, 43, 4993-5000; doi: 10.1039/C3DT52381K
10. "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
11. "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
12. "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

13. "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
14. "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
15. "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
16. "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
17. "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
18. "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
19. "Comparison of hypoelectronic deltahedral ditechneboranes 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
20. "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
21. "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
22. "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
23. "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
24. "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
25. "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
26. "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
27. "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
28. "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
29. "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
30. "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

31. "The prevalence of isocloso deltahedra in low-energy hypoelectronic metalladiboranes with a single metal vertex: manganese and rhenium derivatives" A. Lupan, R.B. King, *Dalton Trans.*, 2012, 41, 7073; doi: 10.1039/c2dt30442b
32. "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.
33. "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
34. "Limited occurrence of isocloso deltahedra with 9 to 12 vertices in low-energy hypoelectronic diferradiborane structures" A. Lupan, R.B. King, *Inorg. Chem.*, 2011, 50, 9571; doi: 10.1021/ic201321f
35. "Computational modelling metal-protein interactions: cisplatin" A. Lupan, A. Kun, R. Silaghi-Dumitrescu, *Metal Elem. Environ. Med. Biol.*, 2010, 10, 199.
36. "PM6 modeling of alpha-helical polypeptide structures" A. Kun, A. Lupan, R. Silaghi-Dumitrescu, *Stud. Univ. Babeş-Bolyai Chem.*, 2010, 55, 265.
37. "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. Viadain, A. Lupan, H. Munier-Lehmann, 2009, EU Patent EP2065476-A1
38. "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. Viadain, 2009, US Patent US2011159480-A1
39. "A mammalian cell-based screening assay to identify inhibitors of alphaviruses" P.O. Viadain, F. Tangy, Y. Jacob, M. Lucas-Hourani, H. Munier-Lehmann, A. Lupan, 2008, Patent wipo: <http://patentscope.wipo.int/search/en/WO2009068998>
40. "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.
41. "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
42. "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
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44. "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
45. "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
46. "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
47. "The shapes of hypoelectronic six-vertex anionic bare boron clusters: Effects of the counterions" R.B. King, I. Silaghi-Dumitrescu, A. Lupan, A. Kun, *Main Group Chem.*, 2005, 4, 291; doi: 10.1080/10241220600798435