

## Articole

1. J.D. Wang et. al. "Conjugated sulfonamides as a class of organic lithium-ion positive electrodes" *Nature Materials* 20 665 (2021) DOI10.1038/s41563-020-00869-1
2. L. Sieuw et. al. "Through-Space Charge Modulation Overriding Substituent Effect: Rise of the Redox Potential at 3.35 V in a Lithium-Phenolate Stereoelectronic Isomer" *Chemistry of Materials* 32 9996-10006 (2020) DOI10.1021/acs.chemmater.0c02989
3. D. Miklik et. al. "Pyrazinacenes exhibit on-surface oxidation-state-dependent conformational and self-assembly behaviours" *Communications chemistry* 4 29 (2021) DOI10.1038/s42004-021-00470-w
4. A. Calborean, T. Murariu, C. Morari "Optimized lead-acid grid architectures for automotive lead-acid batteries: An electrochemical analysis" *Electrochimica Acta* 327 134636 (2021) DOI10.1016/j.electacta.2021.137880
5. A. Calborean, O. Bruj, T. Murariu, C. Morari "Resonance frequency analysis of lead-acid cells: An EIS approach to predict the state-of-health" *Journal of Energy Storage* 27 101143 (2020) DOI10.1016/j.est.2019.101143
6. A. Calborean, T. Murariu, C. Morari "Determination of current homogeneity on the electrodes of lead-acid batteries through electrochemical impedance spectroscopy" *Electrochimica Acta* 320 134636 (2019) DOI10.1016/j.electacta.2019.134636
7. D. Sticlet, C. Morari "Topological superconductivity from magnetic impurities on monolayer NbSe<sub>2</sub>" *Phys Rev. B* 100 075420 (2019) DOI10.1103/PhysRevB.100.075420
8. T. Biter, L. Buimaga-larinca and C. Morari "Weak interactions between tetraphenylporphyrin dimers: A Wannier orbitals study" *Physics Letters A* 384, 126717 (2020) DOI10.1016/j.physleta.2020.126717
9. Buimaga-larinca, L; Morari, C, The effect of translation on the binding energy for transition-metal porphyrines adsorbed on Ag(111) surface, *BEILSTEIN JOURNAL OF NANOTECHNOLOGY*, 10, 706-717, 2019, DOI: 10.3762/bjnano.10.70
10. Murariu, T; Morari, C, Time-dependent analysis of the state-of-health for lead-acid batteries: An EIS study, *JOURNAL OF ENERGY STORAGE*, 21, 87-93, 2019; DOI: 10.1016/j.est.2018.11.011
11. Buimaga-larinca, L; Morari, C, Charge transport pathways in metal porphyrin as interplay between long and short range scattering processes, *NANOTECHNOLOGY*, 30, 045204, 2019, DOI: 10.1088/1361-6528/aaed75
12. Buimaga-larinca, L; Morari, C, Translation of metal-phthalocyanines adsorbed on Au(111): from van der Waals interaction to strong electronic correlation, *SCIENTIFIC REPORTS*, 8, 12728, 2018, DOI: 10.1038/s41598-018-31147-5
13. Calborean, A; Morari, C ; Maldivi, P, Combined Molecular and Periodic DFT Analysis of the Adsorption of Co Macrocycles on Graphene, *JOURNAL OF COMPUTATIONAL CHEMISTRY*, 39, 130-138, 2018, DOI: 10.1002/jcc.25093
14. Morari, C; Appelt, WH; Ostlin, A; Prinz-Zwick, A; Schwingenschlogl, U; Eckern, U; Chioncel, L, Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures, *PHYSICAL REVIEW B*, 96, 205137, 2017, DOI: 10.1103/PhysRevB.96.205137

15. Pawlak, M; Streza, M; Morari, C; Strzalkowski, K; Depriester, M; Chirtoc, M, Quantitative thermal wave phase imaging of an IR semi-transparent GaAs wafer using IR lock-in thermography, MEASUREMENT SCIENCE AND TECHNOLOGY, 28, 025008, 2017, DOI: 10.1088/1361-6501/aa4f69
16. Morari, C; Buimaga-larinca, L; Rungger, I; Sanvito, S; Melinte, S; Rignanese, GM, Charge and spin transport in single and packed ruthenium-terpyridine molecular devices: Insight from first-principles calculations, SCIENTIFIC REPORTS, 6, 31856, 2016, DOI: 10.1038/srep31856
17. Bogdan, M; Floare, CG; Buimaga-larinca, L; Morari, C; Pirnau, A, NMR study and computational assays of meclofenamic Na salt and beta-cyclodextrin inclusion complex, JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY, 85, 111-120, 2016, DOI: 10.1007/s10847-016-0610-7
18. Buimaga-larinca, L; DeNardis, NI; Vernier, PT; Calborean, A; Morari, C, The Effect of the Electric Field on the alpha-GPC Interaction with Au(111) Surface: A First-Principles Study, JOURNAL OF PHYSICAL CHEMISTRY C, 120, 9740-9749, 2016, DOI: 10.1021/acs.jpcc.5b12400
19. Streza, M; Nut, C; Tudoran, C; Bunea, V; Calborean, A; Morari, C, Distribution of current in the electrodes of lead-acid batteries: a thermographic analysis approach, JOURNAL OF PHYSICS D-APPLIED PHYSICS, 49, 055503, 2016, DOI: 10.1088/0022-3727/49/5/055503
20. Chioncel, L; Morari, C; Ostlin, A; Appelt, WH; Droghetti, A ; Radonjic, MM; Rungger, I; Vitos, L; Eckern, U; Postnikov, AV, Transmission through correlated CunCoCun heterostructures, PHYSICAL REVIEW B, 92, 054431, 2015, DOI: 10.1103/PhysRevB.92.054431
21. Morari, C; Beiuseanu, F; Di Marco, I; Peters, L; Burzo, E; Mican, S ; Chioncel, L, Magnetism and electronic structure calculation of SmN, JOURNAL OF PHYSICS-CONDENSED MATTER, 27, 115503, 2015, DOI: 10.1088/0953-8984/27/11/115503
22. Muntean, CM; Bratu, I; Leopold, N; Morari, C; Buimaga-larinca, L; Purcaru, MAP, Subpicosecond surface dynamics in genomic DNA from in vitro-grown plant species: a SERS assessment, PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 17, 21323-21330, 2015, DOI: 10.1039/c4cp05425c
23. Buimaga-larinca L; Morari C, Adsorption of small aromatic molecules on gold: a DFT localized basis set study including van der Waals effects, THEORETICAL CHEMISTRY ACCOUNTS, 133, 1502, 2014, DOI: 10.1007/s00214-014-1502-9
24. Buimaga-larinca, L; Floare, CG; Morari, C, DFT study of the trioxotriangulene derivatives in bulk state, CHEMICAL PHYSICS LETTERS, 598, 48-52, 2014, DOI: 10.1016/j.cplett.2014.03.002
25. Morari, C; Muntean, CM; Tripon, C; Buimaga-larinca, L; Calborean, A, DFT investigation of the vibrational properties of GC Watson-Crick and Hoogsteen base pairs in the presence of Mg<sup>2+</sup>, Ca<sup>2+</sup>, and Cu<sup>2+</sup> ions, JOURNAL OF MOLECULAR MODELING, 20, 2220, 2014, DOI: 10.1007/s00894-014-2220-x
26. Pinzaru, SC; Falamas, A; Dehelean, C; Morari, C; Venter, M, Double Amino Functionalized Ag Nanoparticles as SERS Tags in Raman Diagnostic, CROATICA CHEMICA ACTA, 86, 233-244, 2013, DOI: 10.5562/cca2067
27. Buimaga-larinca, L; Morari, C, Effect of Conformational Symmetry upon the Formation of Cysteine Clusters on the Au(110)-(1 x 1) Surface: A First-Principles Study, JOURNAL OF PHYSICAL CHEMISTRY C, 117, 20351-20360, DOI: 10.1021/jp4072857

28. Bogdan, D; Morari, C, Effect of van der Waals Interaction on the Geometric and Electronic Properties of DNA Nucleosides Adsorbed on Cu(111) Surface: A DFT Study, JOURNAL OF PHYSICAL CHEMISTRY A, 117, 4669-4678, 2013, DOI: 10.1021/jp401041a
29. Buimaga-Iarinca, L; Morari C, Adsorption of cysteine clusters on Au(110)-(1 x 1) surface: a DFT study, RSC ADVANCES, 3, 5036-5044, 2013, DOI: 10.1039/c3ra23214j
30. Morari, C; Bogdan, D, Binding effects of Mn<sup>2+</sup> and Zn<sup>2+</sup> ions on the vibrational properties of guanine-cytosine base pairs in the Watson-Crick and Hoogsteen configurations, JOURNAL OF MOLECULAR MODELING, 18, 4781-4786, 2012, DOI: 10.1007/s00894-012-1480-6
31. Bogdan, D; Morari, C, Electronic Properties of DNA Nucleosides Adsorbed on a Au(100) Surface, JOURNAL OF PHYSICAL CHEMISTRY C, 116, 7351-7359, 2012, DOI: 10.1021/jp210229e
32. Bogdan, D; Isai, R; Calborean, A; Morari, C; Ab initio study of the vibrational properties of single-walled silicon nanotubes, PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES, 44, 1441-1445, 2012, DOI: 10.1016/j.physe.2012.03.008
33. Morari, C; Allmaier, H; Beiuseanu, F; Jurcut, T; Chioncel, L; Electronic structure and magnetic properties of metallocene multiple-decker sandwich nanowires, PHYSICAL REVIEW B, 85, 085413, 2012, DOI: 10.1103/PhysRevB.85.085413
34. Bende, A; Bogdan, D; Muntean, CM; Morari, C, Localization and anharmonicity of the vibrational modes for GC Watson-Crick and Hoogsteen base pairs, JOURNAL OF MOLECULAR MODELING, 17, 3265-3274, 2011, DOI: 10.1007/s00894-011-1002-y
35. Hangan, A; Borodi, G; Filip, X; Tripon, C; Morari, C; Oprean, L; Filip, C, Structure of N-(5-ethyl-[1,3,4]-thiadiazole-2-yl)toluenesulfonamide by combined X-ray powder diffraction, <sup>13</sup>C solid-state NMR and molecular modelling, ACTA CRYSTALLOGRAPHICA SECTION B-STRUCTURAL SCIENCE, 66, 615-621, 2010, DOI: 10.1107/S0108768110039327
36. Morari, C; ; Rungger, I; Rocha, AR; Sanvito, S; Melinte, S; Rignanese, GM, Electronic Transport Properties of 1,1'-Ferrocene Dicarboxylic Acid Linked to Al(111) Electrodes, ACS NANO, 3, 4137-4143, 2009, DOI: 10.1021/nn9012059
37. Morari, C; Bogdan, D; Turcu, I, A first-principles study of pi-conjugated thiol phenothiazine derivatives adsorbed on Au(111) surface, CENTRAL EUROPEAN JOURNAL OF PHYSICS, 7, 332-339, 2009, DOI: 10.2478/s11534-008-0128-8
38. Morari, C, Bond energy and electronic structure in M-bis-terpyridine complexes (M = Os, Co and Ru), PHYSICS LETTERS A, 372, 1885-1889, 2008, DOI: 10.1016/j.physleta.2007.10.078
39. Morari, C; Rignanese, GM; Melinte, S, Electronic properties of 1-4, dicyanobenzene and 1-4, phenylene diisocyanide molecules contacted between Pt and Pd electrodes: First-principles study, PHYSICAL REVIEW B, 76, 115428, 2007, DOI: 10.1103/PhysRevB.76.115428
40. Bogdan, D; Morari, C, Electronic structure and driving forces in beta-cyclodextrin: Diclofenac inclusion complexes, PHYSICS LETTERS A, 366, 454-459, 2007, DOI: 10.1016/j.physleta.2007.02.084
41. Bogdan, D; Morari, C, Theoretical investigation of the normal modes for the ground and first excited states of a realistic retinal chromophore model, PHYSICA SCRIPTA, 73, 447-451, 2006, DOI: 10.1088/0031-8984/73/5/006

42. Morari, C; Bogdan, D, A study of the anharmonic effects on the vibrational spectra of a realistic retinal chromophore model, SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, 61, 1881-1886, 2005, DOI: 10.1016/j.saa.2004.07.017
43. Morari, C; Jaquet, R, Time-dependent reactive scattering for the system  $H+D-2 \leftrightarrow HD+D-$  and comparison with  $H+H-2 \leftrightarrow H-2+H-$ , JOURNAL OF PHYSICAL CHEMISTRY A, 109, 3396-3404, 2005, DOI: 10.1021/jp0462963
44. Bogdan, M; Caira, M; Bogdan, D; Morari, C; Farcas, SI; Evidence of a bimodal binding between diclofenac-Na and beta-cyclodextrin in solution, JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY, 49, 225-229, 2004, DOI: 10.1023/B:JIPH.0000048311.02653.23
45. Pinzaru, SC; Morari, C, Vibrational properties of the free and adsorbed acridone, SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY, 60, 337-342, 2004, DOI: 10.1016/S1386-1425(03)00231-2
46. Morari, CI; Muntean, CM, Numerical simulations of Raman spectra of guanine-cytosine Watson-Crick and protonated Hoogsteen base pairs, BIOPOLYMERS, 72, 339-344, 2003, DOI: 10.1002/bip.10418

#### Carti:

1. C. Morari and R Jaquet: "Quantum Reactive Scattering for Ion-neutral Collisions: The  $H_3^-$  system" pag. 333 in E Krause, W Jäger and M Resch (Eds), "High Performance Computing in Science and Engineering 2004 Transactions of the High Performance Computing Center Stuttgart (HLRS) 2004" Springer-Verlag, Springer Berlin Heidelberg, 2005
2. (BVB-BibliotheksVerbund Bayern FAST-Zugang KOBV Berlin-Brandenburg (Index) Verbundkatalog GBV TIB Hannover (TIBORDER) SWB, Südwestdeutscher Bibliotheksverbund Deutsche Nationalbibliothek) [www.ubka.uni-karlsruhe.de/kvk.html](http://www.ubka.uni-karlsruhe.de/kvk.html)
3. C. Morari „Modelarea transportului electronic in sisteme nanoscopice”, Casa cartii de stiinta, 2007

#### Capitole

1. L Buimaga-Iarinca, D. Marconi, A. Colnita, C. Morari, I. Turcu - Molecular Devices: From Rational Design to Functional Units in Nanotechnologies and Nanomaterials for Various Applications (D. Dascalu ed.), Editura Academiei Romane (2018), ISBN 978-973-27-2954-8
2. C. Morari, L. Buimaga-Iarinca - Van der Waals forces involved in biomolecules interactions with metallic surfaces in Biophysics for Biomedical and Environmental Sciences (M. Florescu ed.), Transylvania University Press, Brasov (2016), ISBN 978-606-19-1768-7

#### Cereri de Brevet

1. METHOD FOR DETERMINING LIFE AND QUALITY OF LEAD-ACID BATTERIES, INVOLVES TRAKING PARAMETER OF CONSTANT PHASE ELEMENT WITH LINEAR DEPENDENCE ON BATTERY, SLOPE OF LINEAR DEPENDENCE OF PARAMETER AND NUMBER OF LOAD CYCLES/DISCHARGE, Patent

Number(s): RO133009-A0, Inventor(s): MORARI I C, BOT A, BUIMAGA-IARINCA L T, MURARIU A T, Patent Assignee Name(s) and Code(s): INSTUTUTUL NAT CERC DEZVOLTARE TEHNOLOGII IZOT MOLEC, Derwent Primary Accession Number: 2019-40690F, International Patent Classification: G01R-031/36

2. METALLIC GRID WITH OPTIMIZED GEOMETRY FOR LEAD-ACID BATTERY POSITIVE ELECTRODE, Patent Number(s): RO132400-A0, Inventor(s): BOT A, BUIMAGA-IARINCA L T, MORARI I C, MURARIU A T, Patent Assignee Name(s) and Code(s): INST NAT CERC-DEZVOLTARE TEHNOLOGII IZOT MOLEC, Derwent Primary Accession Number: 2018-16004X, International Patent Classification: H01M-010/12; H01M-004/73
3. METALLIC GRID FOR POSITIVE ELECTRODES IN ACID-LEAD BATTERIES, OPTIMIZED TO MINIMIZE MATERIAL CONSUMPTION IN MANUFACTURING PROCESS, Patent Number(s): RO132401-A0, Inventor(s): BOT A, BUIMAGA-IARINCA L T, MORARI I C, MURARIU A T, Patent Assignee Name(s) and Code(s): INST NAT CERC-DEZVOLTARE TEHNOLOGII IZOT MOLEC, Derwent Primary Accession Number: 2018-16003Y, International Patent Classification: H01M-010/12; H01M-004/73