CURRICULUM VITAE

PERSONAL DATA:

Name:	Morari Ioan Cristian
Date of Birth:	October 9, 1970
Place of Birth:	Prundu Bârgăului, Romania
Marital Status:	Married with Morari (Pleşca) Dana Brânduşa on January 24, 1991. Son: Morari Andrei Emil, born on November 30, 1992; Daughter: Morari Camelia Maria, born on January 28, 2003
Present Address:	INCDTIM, Str. Donath 67-103, Zip code: 400293, Cluj-Napoca, Romania
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EDUCATION:

1990-1994	Physics Department of *"Babeş Bolyai" University of Cluj-Napoca*, Romania. Degree: "Bachelor of Science". Diploma work: "Theoretical studies on Sr_2 molecule". Supervision: Prof. O. Cozar
1995-1996	Physics Department of *"Babeş Bolyai" University of Cluj-Napoca*, Romania. Degree: "Master of Science" Thesis: "Adsorbtion of the hydrogen on the metals: a study using the electrostatic images method". Supervision: Prof. O. Cozar
1998-2001	Ph.D. work under the guidance of Prof. R. Jaquet, Theoretical Chemistry, Chemistry Department, *University of Siegen*, Germany. Degree: "Doktor der Naturwissenschaften". Thesis: "Time dependent investigation of reactive scattering processes."

EMPLOYMENT:

1996 - 1998	Research Assistant at *National Institute for Research and Development of Isotopic and Molecular Technologies* (NIRDIMT), Cluj-Napoca, Romania.
1998 - 2001	Scientific coworker, Theoretical Chemistry, FB-8, *University of Siegen*, Germany.
2001 - 2004	Research Associate, NIRDIMT, Cluj-Napoca, Romania.
2004 - 2006	Post doc at *Universite catholique du Louvain*, Louvain la Neuve, Belgium.
2006 -	Senior Researcher, NIRDIMT, Cluj-Napoca, Romania.

SKILLS:

Quantum chemistry:	Numerical simmulation of molecular properties using the standard quantum chemistry codes. The investigations that I currently performe include: vibrational spectra, computation of electronic structures and molecular geometries.
Solid state physics:	Application of the ab-initio methods to the study of electronic structures and transport properties on nanodevices. I use both plane waves (ABINIT) and localized basis sets (SIESTA) approaches.
Nanotechnology:	Numerical simulation of strucutral and electronic properties for surface, molecule-surface and interface states. Electronic structure properties and transport properties for metal-molecule-metal systems (TansSIESTA, Smeagol codes).
Fortran programming:	Development of several codes (wavepacket dynamics, density of states for the surface plasmon polariton, post-processing codes for SIESTA). Participation to the ABINIT project. Numerical simulation of transport processes in batteries. Numerical analysis of digital images

BLIOGRAPHIC LIST

I. PhD Thesis PhD in Natural Sciences, University of Siegen, Germany. PhD Thesis: Time- dependent investigations of reactive scattering processes. Siegen, 27 April 2001. Supervisor: Prof. Dr. R. Jaquet. (see: http://www.ub.uni-siegen.de/epub/diss/morari.htm)

II. Publications with referees:

a. Articles and Impact Factor (IF) :

First autor :

1. (IF:2.88) C. Morari, C. Munteanu, Numerical simulations of the Raman spectra of GC Watson-Crick and Hoogsteen Base Pairs, Biopolymers (Biospectroscopy) 72, 339-344 (2003).

2. (IF:1.98) C. Morari, D. Bogdan, A study of the anharmonicity effects on a realistic retinal chromophore Spectrochimica Acta A, 61 (8), 1881-1886 (2005).

3. (IF: 2.77) C. Morari, R. Jaquet Time-dependent reactive scattering for the system H + D2 HD + D2 and comparison with H + H2 H2 + H J. Phys. Chem. A 109 (15), 3396-3404 (2005).

4. (IF: 3.77) C. Morari, G-M. Rignanesse and S. Melinte, Electronic properties of 1-4,dicyanobenze and 1-4,diisocyanidebenzen molecules contacted between two platinum and palladium electrodes: a first-principles study Phys. Rev. B 76, 115428 (2007)

5. (IF: 1.77) C. Morari, Bond energy and electronic structure in M - bis-terpyridine complexes (M=Os, Co and Ru) Physics Letters A 372, 1885-1889 (2008). (IF: 0.91) C. Morari, D. Bogdan and I. Turcu A rst-principles study of -conjugated thiol phenothiazine derivatives adsorbed on Au(111) surface Cent. Eur. J. Phys. 7(2), 332 (2009).

6. (IF: 12.06) C. Morari, I. Rungger, A. Rocha, S. Sanvito, S. Melinte and G-M. Rignanese Electronic transport properties of 1,1-ferrocene dicarboxylic acid linked to Al(111) electrodes ACS Nano Vol. 3 no. 12, 4137-4143 (2009)

7. (IF: 3.77) C. Morari, H. Allmaier, F. Beiuseanu et al. "Electronic structure and magnetic properties of metallocene multiple-decker sandwich nanowires" *Phys. Rev. B* **85(8)**, 085413 (2012)

8. (IF: 1.98) C. Morari, D. Bogdan, C. M. Muntean "Binding Effects of Mn^{2+} and Zn^{2+} Ions on the Vibrational Properties of Guanine-Cytosine Base Pairs in the Watson-Crick and Hoogsteen Configurations" *J. Mol. Model.* **18(11)**, 4781 (2012)

9. (IF: 1.98) C. Morari, C. M. Muntean, C. Tripon, L. Buimaga-Iarinca and A. Calborean "DFT investigation of the vibrational properties of GC Watson-Crick and Hoogsteen base pairs in the presence of Mg^{2+}, Ca^{2+}, and Cu^{2+} ions" *J. Mol. Model.* **20**, 2220 (2014)

10. (IF:2.10) C. Morari, F. Beiuseanu, I. Di Marco, L. Peters, E. Burzo, S. Mican, L. Chioncel "Magnetism and electronic structure calculation of SmN" Journal of Physics:Condensed Matter **27** 15503 (2015)

11. (IF: 4.32) C. Morari, L. Buimaga-Iarinca, S. Sanvito, I. Rungger, S. Melinte, G-M. Rignenese "Charge and spin transport in single and packed ruthenium-terpyridine molecular devices : Insight from first-principles calculations" Scientific Reports **6** 31856 (2016)

Corresponding author :

1. (IF:1.98) S. Cinta, C. Morari, Vibrational properties of the free and adsorbed acridone Spectrochimica Acta A, 60, 337-342 (2004).

2. (IF: 1.03) D. Bogdan, C. Morari Theoretical investigation of the normal modes for the ground and first excited states of a realistic retinal chromophore model Phys. Scripta 109 (15), 3396-3404 (2006)

3. (IF: 1.77) D. Bogdan, C. Morari Electronic structure and driving forces in - cyclodextrin: diclofenac inclusion complexes Phys. Lett. A 366, 454-459 (2007)

4. (IF: 1.98) A. Bende, D. Bogdan, C.M. Muntean, C. Morari Localization and anharmonicity of the vibrational modes for GC Watson-Crick and Hoogsteen base pairs J. Mol. Model 17(12) 3265 (2011)

5. (IF: 4.81) D. Bogdan, C. Morari "Electronic Properties of DNA Nucleosides Adsorbed on a Au(100) Surface" *J. Phys. Chem. C* **116(13)**, 7351 (2012)

6. (IF: 1.52) D. Bogdan, R. Isai, A. Calborean, C. Morari "Ab-initio study of the vibrational properties of single-walled silicon nanotubes" *Physica E* **44(7-8)**, 1441 (2012)

7. (IF: 3.84) L. Buimaga-Iarinca and C. Morari "Adsorption of cysteine clusters on Au(110)-(1X1) surface: a DFT study" *RSC Advances* **3(5)** 5036 (2013)

8. (IF: 2.77) D. Bogdan and C. Morari "Effect of van der Waals Interaction on the Geometric and Electronic Properties of DNA Nucleosides Adsorbed on Cu(111) Surface: A DFT Study" *J. Phys. Chem. A* **117(22)** 4669 (2013)

9. (IF: 4.81) L. Buimaga-Iarinca and C. Morari "Effect of Conformational Symmetry upon the Formation of Cysteine Clusters on the Au(110)-(1 x 1) Surface: A First-Principles Study" *J. Phys. Chem. C* **117(39)** 20351 (2013)

10. (IF: 2.15) L. Buimaga-Iarinca, C. G. Floare and C. Morari "DFT study of the trioxotriangulene derivatives in bulk state" *Chem. Phys. Letters* **598** 48 (2014)

11. (IF: 2.01) L. Buimaga-Iarinca and C. Morari "Adsorption of small aromatic molecules on gold: a DFT localized basis set study including van der Waals effects" *Theoretical Chemistry Accounts* **133** 1502 (2014)

12. (IF: 2.72) M. Streza, C. Nuţ, C. Tudoran, V. Bunea, A. Calborean, C. Morari "Distribution of current in the electrodes of lead-acid batteries: a thermographic analysis approach" *The Journal of Physics D* **49(5)** 055503 (2016)

13. (IF: 4.81) L. Buimaga-Iarinca, N. Ivosevic DeNardis, P. T. Vernier, A. Calborean, and C. Morari "The Effect of the Electric Field on the α-GPC Interaction with Au(111) Surface: A First-Principles Study" *J. Phys. Chem. C* **120 (18)**, 9740 (2016)

Coauthor :

1. (IF:1.40) V. Chis, M. Brustolon, C. Morari, O. Cozar, L. David, Experimental and theoretical structural parameters of the glycine CH2 -NH2 radical, J. Mol. Struc. 482-483, 283 (1999).

2. (IF:1.75) S. Cinta, C. Morari, E. Vogel, D. Maniu, M. Aluas, T. Iliescu, O. Cozar, W. Kiefer, Vibrational studies of B6 Vitamin, Vibrational Spectroscopy 19, 329 (1999).

3. (IF:1.40) M. Bogdan, M. Caira, D. Bogdan,C. Morari and S. Farcas Evidence of a bimodal binding between diclofenac-Na and beta-cyclodextrin in solution J. Incl. Phenom and Macrocyclic Chemistry 49 225 (2004)

4. (IF:0.61) S. Cinta Pinzaru et. al "Double Amino Functionalized Ag Nanoparticles as SERS Tags in Raman Diagnostic" *Croatica Chemica Acta* **86(3)** 233 (2013)

5. (IF:4.42) C. Muntean, I. Bratu, N. Leopold, C. Morari et. al, "Subpicosecond surface dynamics in genomic DNA from in vitro-grown plant species: a SERS assessment" *Phys Chem Chem Phys* **17 (33)** 21323-21330 (2015)

6. (IF:3.77) L. Chioncel, C. Morari, et. al, "Transmission through correlated Cu_nCoCu_n heterostructures" *Phys Rev. B* **92 (5)** 054431, (2015)

II. Books and proceedings (selected):

1. C. Morari, R. Rohse, R. Jaquet, "Time-dependent reactive scattering for ion-neutral collisions in: E. Krause, W. Jager (Eds.) High Performance Computing in Science and Engineering 2000", (Springer-Verlag, Berlin, 2001) pag 207; ISBN 978-3-642-56548-9.

2. C. Morari and R. Jaquet, "Quantum Reactive Scattering for Ion-neutral Collisions: The H3 - system" in: E. Krause, W. Jger and M. Resch (Eds.) "High Performance Computing in Science and Engineering 2004 Transactions of the High Performance Computing Center Stuttgart (HLRS) 2004" (Springer Berlin Heidelberg, 2005) pag 333-347 ISBN 978-3-540-22943-8 (Print) 978-3-540-26589-4 (Online)

3. C. Morari "Modelarea transportului electronic in sisteme nanoscopice (Modeling the electronic transport in nanoscopic systems)", (Casa Cartii de Stiinta, Cluj-Napoca, 2007; ISBN 978-973-133-074-7)

Researcherid page: www.researcherid.com/rid/C-2131-2011
Researchgate page: www.researchgate.net/profile/Cristian_Morari/

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