



PERSONAL INFORMATION

## Morari Ioan Cristian

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Researcherid page: [www.researcherid.com/rid/C-2131-2011](http://www.researcherid.com/rid/C-2131-2011)

Researchgate page: [https://www.researchgate.net/profile/Cristian\\_Morari](https://www.researchgate.net/profile/Cristian_Morari)

Sex M | Date of birth 9/10/1970 | Nationality Romanian

WORK EXPERIENCE

2006 -

### Senior Researcher

*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*

Research areas: molecule-surface interaction; surface and interface phenomena; electronic transport; characterization and design of batteries for industrial applications

2004 - 2006

### Post-doctoral Researcher

*Universite Catholique du Louvain, Louvain la Neuve, Belgium*

Numerical simulation of transport phenomena at nanoscopic scale; theoretical molecular electronics

2001 - 2004

### Research Associate

*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*

Theoretical investigation of molecular properties: vibrational analysis, intermolecular interaction and molecular docking

1998 - 2001

### Scientific coworker

*Theoretical Chemistry, FB-8, University of Siegen, Germany*

PhD student: development of the FORTRAN code to be used for the simulation of time dependent scattering in chemical reactions

1996 - 1998

### Research Assistant

*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*

Theoretical and experimental investigation of molecular properties (mainly IR and Raman spectra)

EDUCATION AND TRAINING

1998 - 2001

### Doktor der Naturwissenschaften

*Theoretical Chemistry Department, University of Siegen, Germany*

- Thesis: Time dependent investigation of reactive scattering processes. Ph.D. work under the guidance of Prof. R. Jaquet

1996 - 1998

### Master of Science

*Physics Department of "Babes Bolyai" University of Cluj-Napoca, Romania*

- Thesis: Adsorption of the hydrogen on the metals: a study using the electrostatic images method. Supervision: Prof. O. Cozar

1990 - 1994

### Bachelor of Science

*Physics Department of "Babes Bolyai" University of Cluj-Napoca, Romania.*

- Diploma work: Theoretical studies on Sr<sub>2</sub> molecule, Supervision: Prof. O. Cozar.

PERSONAL SKILLS

Mother tongue(s) Romanian

Other language(s)	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C1	C1	C1	C1
French	C1	C1	C1	C1	C1
German	A2	A2	A2	A2	A2

Levels: A1/A2: Basic user - B1/B2: Independent user - C1/C2 Proficient user

#### SCIENTIFIC SKILLS

Quantum Technologies	Computational characterization of granular aluminum as superconducting qubits material; ab-initio calculations of electronic properties of molecular Qubits.
Quantum chemistry and Nanotechnology	Numerical simulation of molecular properties using the standard quantum chemistry codes. The investigations that I currently performed include: vibrational spectra, computation of electronic structures and molecular geometries. Numerical simulation of structural and electronic properties for surface, molecule-surface and interface states. Electronic structure properties and transport properties for metal-molecule-metal systems (TansSIESTA, Smeagol codes).
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.
Energy storage	Investigation of batteries by electrochemical impedance spectroscopy (EIS). Numerical simulation of structural & redox processes in batteries (using GAMESS and SIESTA).
Programming and Numerical modeling	Development of several codes (wavepacket dynamics, post-processing codes for SIESTA). Participation to the ABINIT project. Numerical simulation of transport processes in nanostructures.

#### ADDITIONAL INFORMATION

Membership  
European Biophysics Society  
Romanian Physics Society

Referent for  
J. Chem. Phys, J. Mol. Struct., J Mol. Mod, Sci Rep.