



**Anexa nr. 1 – Cerere de premiere\***

**1. Candidat**

**Nume: Morari**

Nume anterioare (dacă este cazul):

**Prenume: Ioan Cristian**

Doctor din anul (se prezintă copie a diplomei de doctor sau echivalent): 2001

Poziția ocupată: Senior Researcher I

Instituția: National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM) Cluj-Napoca

Telefon mobil: .

Adresa de e-mail: \_\_\_\_\_

**2. Ediția “Gala Cercetării Românești”: 2024**

**3. Premiul și categoria pentru care aplică (individual sau echipă de cercetare):**

**"Nicolae Vasilescu Karpen" Award in the Energy and Advanced Materials – Research Team**

**4. Lider de echipă, dacă este cazul: Leader of Group of Structural and Computational Analysis**

**5. Componenta echipei de cercetare, dacă este cazul (numele membrilor echipei, poziția ocupată, anul ultimei diplome acordate):**

1. Cristian Morari – PhD in Physics since 2001, leader of the Structural and Computational Analysis Group, INCDTIM Cluj-Napoca
2. Luiza Buimaga-Iarinca – Senior Researcher, PhD in Physics since 2011, member of the Structural and Computational Analysis Group, INCDTIM Cluj-Napoca
3. Gheorghe Borodi – Senior Researcher, PhD since 1999, member of the Structural and Computational Analysis Group, INCDTIM Cluj-Napoca



6. O descriere a celor mai importante realizări științifice din ultimii 5 ani (max. 4 pag., format A4, caractere Times New Roman, 12 puncte, spațiere între linii de 1,5 și margini de 2 cm)\*\*.

Our Group is focused on the **computational evaluation of material properties**, such as structural analysis, electronic structure and properties, diffusion and transport calculations, by using **numerical models and methods** from Density Functional Theory (DFT) to Molecular Dynamics (MD). Through tight collaborations with excellent international groups of experimentalists, our team shares expertise in modeling and assessing a large variety of materials, from molecules, to surfaces and bulk structures.

In the past 5 years, the Group focuses on **two main directions**: (i) support experimentalist scientists into developing **new materials for improved batteries capacity**, and (ii) the study of **materials dedicated to quantum technologies**, and in particular to the fabrication of superconducting qubits.

### **Materials Chemistry for improved batteries capacity**

Our research **high quality and excellent collaboration** with high profile international research groups is highlighted by the publication in Jan 2021 in **Nature Materials** of a study that **extend the chemical space of organic Li-ion positive electrode materials with a class** of conjugated sulfonamides (CSAs). This class of organic Li-ion positive electrode materials challenges the realm of the inorganic battery cathode, as this first generation of CSA chemistries already displays gravimetric energy storage metrics comparable to those of the stereotypical LiFePO<sub>4</sub>. (<https://doi.org/10.1038/s41563-020-00869-1>)

Group Leader is the initiator of the **Agreement of Cooperation** between **l'Université catholique de Louvain (UCL)** Louvain-la-Neuve, Belgium and **INCDTIM Cluj-Napoca**, in which UCL firmly agreed to support the research activities through performing the experiments, i.e. the molecular synthesis and characterization (the signed Agreement is available upon request).

This collaboration led to explaining and/or predicting the role of the chemical compounds used in experiments, and also to offering computational models that explain the overall properties of MOF-based batteries and in the **past 5 years** resulted in **8 publications with a total impact factor over 150**.

We recall **Nature Materials** (IF 41.2) <https://doi.org/10.1038/s41563-020-00869-1>, **Advanced Science** (IF 15.1) <https://doi.org/10.1002/adv.202200924>, **Energy&Environmental Science** (IF 32.5)



<https://doi.org/10.1039/D2EE00566B>, ACS Energy Letters (IF 22)

<https://doi.org/10.1021/acscenergylett.1c02571>, or Science Advances (IF13.6)

<https://doi.org/10.1126/sciadv.adg6079>

Group Leader is also the **initiator of the cooperation between INCDTIM and SC ROMBAT SA** (Agreement of collaboration nr 646/24.11.2017), which is the **main producer of lead-acid batteries in Romania**. In this framework they successfully implemented the activities of the Joint Applied Research Project “The improvement of the manufacturing technology of lead-acid batteries to be used for start-and-stop automobiles”, contract PN-II-PT-PCCA-2013-4-248 (over 40 researchers involved between 2014–2017, from which 3 new researchers were employed by INCDTIM). During the implementation of this project and afterwards, this scientific effort output into the publication of **8 papers** (from which 3 in Journal of Energy Storage – IF 9.4 and 2 in Electrochimica Acta–IF 6.6). The computational models proposed within this project resulted in **5 national patent requests** to Romanian Office for Inventions and Trademarks according to Derwent Innovations Index and also into a **method of testing the current distribution in the electrodes** of lead-acid battery - see for a description:

<https://doi.org/10.1088/0022-3727/49/5/055503>

### **In the field of new materials for Quantum Technologies,**

**Dr Luiza Buimaga-Iarinca** is the coordinator of the **Romanian Quanterra QuCos team**, that in the **past 5 years** has the role to offer theoretical support to the experimental and industrial partners that form the QuCos Consortium <https://qucos.eu/>.

We stress that this is the first time when a Romanian team is included in such an elitist list, since 12 QuantERA projects only were funded over the entire EU in 2019 Call <https://www.quanterra.eu/calls-for-proposals/funded-projects-call-2019/97-qucos>.

This collaboration resulted in a better understanding of **aluminum-based Josephson junctions**, as proved by the published papers (<https://doi.org/10.48550/arXiv.2302.09192>, just accepted at **Nature Physics** and <https://doi.org/10.48550/arXiv.2306.04112>, just accepted at **Phys Rev B**).

This joint-research expanded into collaborative research with other QuantERA teams, such as SIUCs team from Barcelona, led by Dr Pol Forn Diaz. Transport calculations through large scale models, over 5000 atoms are carried out in collaboration with the group led by Dr. Jared Cole, RMIT, Australia.



For her work **Dr. Luiza Buimaga-Iarinca** was awarded in 2016 a **Special Mention and a Diploma of Excellence for Physics "Young Researchers in Science and Engineering"**, offered by dr. Rada Mihalcea (Michigan State University) to „young researchers in the field of science and engineering who, through their work, have demonstrated excellence and made extraordinary contributions in their field”<https://primariaclujnapoca.ro/evenimente/tinerii-cercetatori-premiul-pentru-stiinta-si-inginerie/>.

In addition to the above-mentioned results, in the past few years, the Group was involved in **many international collaborations in material chemistry area**.

The collaboration with Prof. Thomas Jung’s group, from **Basel University, and PSI, Switzerland** aim at **exploring the quantum states** and the structure-function correlations **for a broad spectrum of functionalized molecules**. This collaboration spans over the **past 5 years** and resulted into high impact research, published in *Comm.Chem.* <https://doi.org/10.1038/s42004-021-00470-w>, in *J PhysChemLett* <https://doi.org/10.1021/acs.jpcclett.2c01592>, or in *PhysChemC* <https://doi.org/10.1021/acs.jpcc.3c03325>.

Based on these joint research studies, an **US patent** was published in April 2023 (Device for capturing free atoms or molecules or clusters or ions in quantum well structure, includes support layer of conductive or insulating material, conductive layer deposited on support layer and quantum well structure fabricated on conductive layer) - [US20230107661\(A1\)](https://patents.google.com/patent/US20230107661A1).

We also mention the collaboration with Dr. Liviu Chioncel’ group (Lehrstuhl für Theoretische Physik III, Institut für Physik, **Universität Augsburg, Germany**). In this framework our groups jointly addressed, for example, Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures, in *PhysRevB* <https://doi.org/10.1103/PhysRevB.96.205137> or *Magnetism and electronic structure calculation of SmN*, in *J Phys:Condens Matter* <https://doi.org/10.1088/0953-8984/27/11/115503>.

**In the field of computational design of new materials**, Group Leader was the receiver of another IDEI grant (project PN-III-P4-IDPCE-2016-0217) whose completion was evaluated as A+. The results of this grant were published in high ranked journals, from which we mention *Nanotechnology* <https://doi.org/10.1088/1361-6528/aaed75>, *Scientific Reports* and *Beilstein J. Nanotechnol* <https://doi.org/10.1038/s41598-018-31147-5> and <https://doi.org/10.3762/bjnano.10.70>.



To date, **the total amount of funds attracted or managed by our Group** is approx. **1.700.000 euro**, from which approx. 920.000 euro represents competitional research grants and approx. 770.000 euro came from intra-institutional grants (7 stages of NUCLEU program in INCDTIM between 2009-2023).

Group leader's research resulted in more than **60 published works**, according to WoS, with an **overall impact factor IF > 380**. Only in the **last five years** Dr. Cristian Morari published a number of papers with an impact factor **IF ~ 240**. According to WoS, in the past 5 years 4 papers were above the 84<sup>th</sup> percentile of **highly cited papers**, out of which 2 papers were in the 98<sup>th</sup> percentile of citations.



7. Curriculum Vitae narativ al candidatului “individual” sau al fiecărui membru al echipei de cercetare, în cazul candidatului “echipă de cercetare”, din care să reiasă rezultatele activității de cercetare din ultimii 5 ani, conform indicatorilor cantitativi din Anexa nr. 2 la regulament și criteriilor de evaluare calitativă prevăzute în Anexa nr. 3 la regulament.

### **Curriculum Vitae**

**DR. CRISTIAN MORARI** (male, 53) works as senior researcher at INCDTIM since 2006; has expertise in numerical simulations of structural and electronic properties for surface, molecule-surface and interface states, ab-initio study of electronic structure and electronic transport at nanoscale, complemented by programming skills.

Brainmap: <https://www.brainmap.ro/ioan-cristian-morari>

Scholar: <https://scholar.google.ro/citations?user=tDUGEQ0AAAAJ&hl=en&oi=ao>

Orcid: <https://orcid.org/0000-0003-1989-3278>

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

### **Education**

[27.04.2001] Ph.D. in Natural Sciences, University of Siegen, Germany.

Thesis: "Time dependent investigation of reactive scattering processes"

[1995-1996] Master in Science in Atomic and Molecular Physics, UBB Cluj Napoca

[1991-1994] Physics Faculty, UBB, Cluj-Napoca

### **Professional Experience**

[2006 - ] Senior Researcher, INCDTIM Cluj-Napoca, Romania. Group leader for Laboratory of manufacturing and testing electrodes for batteries; Implementation and development of the research activities in the field of molecular electronics, nanotechnology and energy storage.

[2014] Post-doctoral fellow (4 months) at Augsburg University, Germany; theoretical study of transport properties of nanostructures

[2004 - 2006] Post-doctoral fellow (Belgian F.R.S. – F.N.R.S.), UCL, Louvain-la-Neuve, Belgium. Ab-initio simulations in molecular electronics.

Work jointly with the ABINIT group in Louvain la Neuve ([www.abinit.org](http://www.abinit.org)) and the SMEAGOL group ([www.smeagol.tcd.ie/index.html](http://www.smeagol.tcd.ie/index.html)).





[2001 - 2004] Senior Researcher, ITIM Cluj-Napoca, Romania. DFT study of electronic structure, vibrational properties of organic molecules by using quantum chemistry.

[1998 – 2001] Scientific coworker, (Theoretical Chemistry) FB-8, University of Siegen, Germany. PhD on the theoretical study of reactive ion-molecule scattering

[1996 - 1998] Research Assistant, ITIM Cluj-Napoca, Romania

### Key qualifications

#### [Research Topics]

atomic and molecular physics, quantum chemistry, computational physics, solid state physics, molecular electronics, nanotechnology, energy storage.

#### [Tools]

Fortran 77-95 programming under UNIX/Linux operating systems, parallel computing.

#### Code development:

Wavepacket dynamics for ion-molecule collisions [J. Phys. Chem. A 109 (15), 3396 (2005)];

Implementation of the Wannier orbitals (via WanT code) in ABINIT (see [www.abinit.org](http://www.abinit.org));

DMFT interface between DMFT/EMTO code from Augsburg University and Smeagol and the implementation of correlation capabilities in Smeagol - Phys Rev. B 92 (5) 054431, (2015).

([www.tcd.ie/Physics/Smeagol/index.html](http://www.tcd.ie/Physics/Smeagol/index.html))

User of several computational chemistry codes – such as GAMESS, SIESTA, ABINIT, GULP

### Scientific output

[Total no of ISI papers]: **62** indexed in WoS (main author for 66%: first author – 23%; last/corresponding author – 42%) – see Papers list

[Total impact factor]: **366.8**

[Times cited] ([www.isiwebknowledge.com](http://www.isiwebknowledge.com)): over **700**; Google Scholar: **over 945**

H=**18** (Google scholar) and **16** (web of science)

### Funds

Project leader for IDEAS grant (project PNCDI III - P4 - ID-PCE 2020-0824 Financed by UEFISCDI with 1200000 RON (approx. 240000 Euro); project duration: 36 months



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Project leader for IDEAS grant (project PN-III-P4-IDPCE-2016-0217) whose completion was evaluated as A+; Financed by UEFISCDI with 850000 RON (approx. 210000 Euro); project duration: 30 months

Project leader for PCCA grant (project PN-II-PT-PCCA-2013-4-1226). Over 40 researchers involved. Financed by UEFISCDI with 1250000 RON (approx. 310000 Euro); project duration: 39 months.

Co-investigator for ERANET-QUANTERA-2019-QuCos (2020 – 2023) - Funded through Horizon2020, program P3-3.2 Horizon 2020-Quanterra H2020. Total value is over 1400000 Euro (national and private funds) out of which Romanian Partner requested 122000 Eu.

Project leader for MCT project PN-III-P1-1.1-MCT-2018-0011, Funded by UEFISCDI with 5845 RON (approx. 1200 Euro) for 2 weeks visit of a Romanian young researcher from Diaspora

Coordinator of 7 stages of NUCLEU project in INCDTIM during 2008-2023

**Patent requests:** 6 patents requested at the Romanian State Office for Inventions and Trademarks; 1 patent requested at United States Patent and Trademark Office – see Patent List

**Referee:** J Phys Chem A-C, Phys Chem Lett, Phys Rev., Phys Chem, Nature

**Evaluator and Supervising Evaluator** for UEFISCDI in Material Science TE 2021

### Invited Talks

**[29.07.2010] invited talk** ACIT Workshop, “*Electronic transport in organometallic compounds*” Augsburg University (Germany);

[www.physik.uni-augsburg.de/~chioncli/acit-html/aktivitaeten/ACIT\\_ES-2010.html](http://www.physik.uni-augsburg.de/~chioncli/acit-html/aktivitaeten/ACIT_ES-2010.html)

**[04.11.2019] invited talk:** “Ab-initio methods in electrochemistry” Université catholique de Louvain, Louvain-la-Neuve, Belgium, Energy Materials Laboratory

Joint invited presentation with E. Csapo-Martinescu from SC ROMBAT SA – at **EuroNanoForum 2019** (June 12). See the official Rombat brochure, RombaTime, 10-th ed.

### Books

C. Morari and R Jaquet: “Quantum Reactive Scattering for Ion-neutral Collisions: The H<sub>3</sub>–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

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 978-3-64256548-9.





## **Curriculum Vitae**

**LUIZA BUIMAGA-IARINCA**, 42 years, computational scientist with PhD in Physics

### **Profile addresses:**

Brainmap: <https://www.brainmap.ro/luiza-buimaga-iarinca>

Scholar: <https://scholar.google.ro/citations?user=piUqvS4AAAAJ&hl=ro>

Publons: <https://publons.com/researcher/1361338/luiza-buimaga-iarinca/>

**Scientometric indicators:** Main author/co-author for 31 indexed publications and 23 scientific communications at international conferences according to WoS (2 awarded, 8 oral communications); 2 Invited Lectures; Co-author for 3 patent requests indexed in Darwent Patent Index.

H=9 ian 2024 according to WoS and H=11 according to Google Scholar. 313 citations according to Google Scholar (231 according to WoS).

### **Information about the degrees and diplomas:**

2008-2011 PhD in Physics - Physics Department, UBB, Cluj-Napoca, Romania

2004-2005 MSc. in Biophys. and Medical Physics - Physics Department, UBB, Cluj-Napoca, Romania

2000-2004 BSc. in Physics - Physics Department, UBB, Cluj-Napoca, Romania

### **Information about the professional experience and jobs:**

2011- present Researcher in Quantum Technologies Group and in the Department of Molecular and Biomolecular Physics, INCDTIM, Cluj-Napoca, Romania

2008-2011 PhD Student - Physics Department of Babes-Bolyai University, Cluj-Napoca, Romania.

2006-2011 Research Assistant - Department of Molecular and Biomolecular Physics, INCDTIM, Cluj-Napoca, Romania

### **Research visits**

July - August 2019 - Visiting researcher in NANOLAB at Basel University, Switzerland

November 2018 - Visiting researcher in the Photon Science Department of PSI, Switzerland

August 2018 - Visiting researcher at the LMN, Paul Scherrer Institute Switzerland

February 2018 - Visiting researcher in NANOLAB at Basel University, Switzerland

September 2017 - Visiting researcher at KIT Karlsruhe, Germany

November 2016 - Visiting researcher at the LMN, Paul Scherrer Institute, Switzerland



### **Job-related skills**

**Computational nanotechnology/physics:** Application of the ab-initio methods in the study of electronic structures of organic molecules interacting with metallic surfaces (SIESTA package); Transport calculations; Nanostructures self-assembly on metallic surfaces.

**Computational chemistry:** Molecular docking on host-guest systems.

**Data processing:** C, C++, Python, Matlab on Linux or Windows.

**Data editing:** Microsoft Office, Latex, Gimp, Mercury, VMD, Chimera, Xmgrace, wxMacMolPlt, etc

### **Awarded Grants**

ERANET-QUANTERA-2019-QuCos (2019) - Quantum Computation with Schrödinger cat states  
Funded by UEFISCDI through program P3-3.2 Horizon 2020-Quantera H2020.

MolSpin2018 COST Action: CA15128, project number: 40920 - The role of vdW forces into the co-adsorption mechanism of FePC and MnPC on Au(111). Funded by European Cooperation in Science and Technology Agency.

PN-III-P1-1.1-MC-2017-1634 - Surface Supported Supramolecular 'Chemistry': Understanding the critical influence of minute interaction forces in their complex balance by DFT—short term mobility, funded by UEFISCDI Romania.

PN16-30-02-01-2016 Coordinator of the micro-project "Computational approach of the specificity of phthalocyanine derivatives adsorption on the noble metal surfaces" within NUCLEUS Project: "Micro- and nano- fabrication techniques dedicated to the development of molecular thermoelectric devices and sensors based on graphene".

PN-II-BD-PCE-2008-1-386 - (2008-2011). Analysis of cellular fluctuations – doctoral grant.

### **Professional Awards**

(1) Diploma of Excellence for Physics (with Special Mention) at the national contest "Young Researchers in Science and Engineering", 2<sup>nd</sup> edition (2016)

(2) ICPAM-9 Sponsor's Prize Received at ICPAM2012, Iasi, Romania

**Invited talks:** Special Seminar "Surface Supported Supramolecular 'Chemistry': Understanding the critical influence of minute interaction forces in their complex balance by DFT modeling", on Feb 15, 2018, in Seminarzimmer 4.1, Department of Physics, University of Basel, Switzerland (WUR=106) and an Invited Talk: "Molecule-surface interaction: a numerical simulation point of view", Sep 15,



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2017, at Physikalisches Institut, Room 4.03, **Karlsruher Institut für Technologie**, Karlsruhe, Germany (WUR=232).

**International visibility:** Referent for J. Chem. Phys, J. Mol. Struct., J Mol. Mod; Sci Rep;

Evaluator for European Comision in EIC Pathfinder OPEN 2022, HORIZON-EUROHPC-JU-2021-COE; Evaluator for MSCA Admire Call 2022; Evaluator for UEFISCDI PTE call 2021

**Other relevant information:** As member of Romanian Quantum Network (<https://roqnet.ro/team/>) Dr Luiza Buimaga-Iarinca was involved into the organisation of the first European Quantum Future Academy <http://roqnet.ro/qfa2020/> and also into the organization in Romania of all European Quantum Week <https://eqw.qt.eu/eqw-education> and World Quantum Day <https://worldquantumday.org/events/> events since 2020.



## Curriculum Vitae

**GHEORGHE BORODI**, 74 years, XRD specialist scientist with PhD in Physics

Profile addresses:

<https://scholar.google.com/citations?user=L4jSDUgAAAAJ&hl=en>

<https://orcid.org/0000-0003-4915-4169>

Scopus Author ID: 6701480916

### Scientometric indicators:

238 ISI articles, 3570 citations without self-citations, Hirsch index 35 according to Scopus

Vast experience in solving crystal structures from both single crystals and powders diffraction, he has been determined many dozens of crystal structures. Some of the solved structures had almost 100 non-hydrogenoid atoms, such as the inclusion complexes with beta Cyclodextrin and for which there are only about 8 solved structures from powders diffraction, some of them are determined by a member of the project team.

### PROFESSIONAL EXPERIENCE

Period: 1973-present Employer: National Institute for Research and Development of Isotopic and Molecular Technologies (INCDTIM) Cluj-Napoca, Romania Scientific Researcher I.

Since 1973, Physicist, Scientific Researcher, CSIII,

Responsibilities: X-ray Powder Diffraction, X-ray Single Crystal Diffraction, Small-Angle X-ray Scattering, X-ray Diffraction on Thin Films.

### EDUCATION AND TRAINING

Period: 1992-1998: Babeș-Bolyai University Cluj-Napoca, Romania, Faculty of Physics Ph.D. studies in Materials Physics Thesis Title: Structural Characterization by X-ray Diffraction of Oxide and Chalcogenide Compounds. Degree Obtained: Ph.D. Diploma with Distinction (Summa Cum Laude)

Period: 1967-1972: Babeș-Bolyai University Cluj-Napoca, Romania, Faculty of Physics, Specialization: Solid State Physics Degree Obtained: B.Sc. Diploma

### PROFESSIONAL SKILLS

Small-Angle X-ray Scattering: determination of specific surfaces, pore sizes, and size distribution; Calculation of electron energy bands in solids; X-ray Diffraction for amorphous compounds: radial distribution function; X-ray Diffraction on crystalline powders: qualitative and quantitative phase analysis; Microstructural analysis (crystallite sizes and lattice distortions, lattice defects), evaluation



of crystallinity degree; X-ray Diffraction on thin films: reflectivity measurements, reciprocal space mapping, pole figures; Ab initio determination of crystal structures from powders: indexing, obtaining the structural model, Rietveld refinement; Complete determination of crystal and molecular structures from single crystals; The mentioned diffraction methods have been applied to various classes of materials: semiconductors, superconductors, perovskites, oxide materials, catalysts, metallic compounds, graphene, magnetic compounds, pharmaceutical compounds, inclusion complexes, MOFs, etc.

**Other mentions:** Teaching activities: course on Diffractometric Methods, seminar on Solid-State Physics.



8. Lista publicațiilor candidatului "individual" sau a fiecărui membru al echipei de cercetare, în cazul candidatului "echipă de cercetare", cu evidențierea publicațiilor relevante ale candidatului în ultimii 5 ani și a publicațiilor comune ale membrilor unei echipe de cercetare în cazul candidatului "echipă de cercetare". Se menționează și un link al paginii web unde se regăsesc publicațiile candidatului.

The full list of paper can be seen at

<https://scholar.google.ro/citations?user=tDUGEQ0AAAAJ&hl=en&oi=ao>

The following list comprise only selected papers published within the **past 5 years, related to the topic** of the award.

Cumulative AIS (31 ian 2024 - 31 ian 2019) according to WoS = **54.407**;

Cumulative (31 ian 2024 – 31 ian 2019) AIS including *just accepted manuscripts* = **65.543**

IF	AIS	Quart	<a href="https://www.webofscience.com/wos/author/rid/C-2131-2011">https://www.webofscience.com/wos/author/rid/C-2131-2011</a>	Year
19.5	10.165	Q1	<i>just accepted</i> in <b>Nature Physics</b> Observation of Josephson Harmonics in Tunnel Junctions, Dennis Willsch, Dennis Rieger, Patrick Winkel, Madita Willsch, Christian Dickel, Jonas Krause, Yoichi Ando, Raphaël Lescanne, Zaki Leghtas, Nicholas T Bronn, Pratiti Deb, Olivia Lanes, Zlatko K Minev, Benedikt Dennig, Simon Geisert, Simon Günzler, Sören Ihssen, Patrick Paluch, Thomas Reisinger, Roudy Hanna, Jin Hee Bae, Peter Schüffelgen, Detlev Grützmacher, <b>Luiza Buimaga-Iarinca</b> , <b>Cristian Morari</b> , Wolfgang Wernsdorfer, David P DiVincenzo, Kristel Michielsens, Gianluigi Catelani, Ioan M Pop <a href="https://doi.org/10.48550/arXiv.2302.09192">https://doi.org/10.48550/arXiv.2302.09192</a>	2024
3.7	0.469	Q2	<i>Just accepted</i> in <b>Phys Rev B</b> Hydrogen crystals reduce dissipation in superconducting resonators, Francesco Valenti, Andrew N Kanagin, Andreas Angerer, <b>Luiza Buimaga-Iarinca</b> , <b>Cristian Morari</b> , Jörg Schmiedmayer, Ioan M Pop, <a href="https://doi.org/10.48550/arXiv.2306.04112">https://doi.org/10.48550/arXiv.2306.04112</a>	2024
6.6	0.917	Q1	<b>Electrochimica Acta</b> . Comparative study of the vibrational contributions to electrochemical potential, in Na <sub>2</sub> -Mn-DOBDC and	2024





			Li <sub>2</sub> -Mn-DOBDC electrodes, <b>C Morari, L Buimaga-Iarinca, C Tripon, RVF Turcu</b> , <a href="https://doi.org/10.1016/j.electacta.2023.143493">https://doi.org/10.1016/j.electacta.2023.143493</a>		
3.7 nici nu e autor	0.827	Q2	<b>The Journal of Physical Chemistry C</b> , Self-Assembly of N-Rich Triimidazoles on Ag (111): Mixing the Pleasures and Pains of Epitaxy and Strain, Aisha Ahsan, Xing Wang, Rejaul Sk, Mehdi Heydari, <b>Luiza Buimaga-Iarinca</b> , Christian Wäckerlin, Elena Lucenti, Silvio Decurtins, Elena Cariati, Thomas A Jung, Ulrich Aschauer, Shi-Xia Liu, <a href="https://doi.org/10.1021/acs.jpcc.3c03325">https://doi.org/10.1021/acs.jpcc.3c03325</a>	2023	
	13.6	5.404	Q1	<b>Science Advances</b> . Revealing the reversible solid-state electrochemistry of lithium-containing conjugated oximates for organic batteries, Jiande Wang, Petru Apostol, Darsi Rambabu, Xiaolong Guo, Xuelian Liu, Koen Robeyns, Mengyuan Du, Yan Zhang, Shubhadeep Pal, Robert Markowski, Fabio Lucaccioni, Alae Eddine Lakraychi, <b>Cristian Morari</b> , Jean-François Gohy, Deepak Gupta, Alexandru Vlad, <a href="https://doi.org/10.1126/sciadv.adg6079">https://doi.org/10.1126/sciadv.adg6079</a>	2023
	6.6	0.917	Q1	<b>Electrochimica Acta</b> , On the contribution of phonons to electrochemical potential of Li-ion metalorganic frameworks, <b>Morari, C.; Buimaga-Iarinca, L.</b> Turcu, R. V. F., <a href="https://doi.org/10.1016/j.electacta.2022.141734">https://doi.org/10.1016/j.electacta.2022.141734</a>	2023
	9.4 nu e autor pp	1.169	Q1	<b>Journal of Energy Storage</b> , Leaf and hexagonal grid designs for lead-acid battery. An EIS analysis, Calborean, Adrian; Bruj, Olivia; <b>Morari, Cristian</b> , <a href="https://doi.org/10.1016/j.est.2022.105933">https://doi.org/10.1016/j.est.2022.105933</a>	2022
	1.7	0.289 Q4	Q4	<b>Theoretical Chemistry Accounts</b> , Calculation of infrared spectra for adsorbed molecules from the dipole autocorrelation function, <b>Buimaga-Iarinca, Luiza; Morari, Cristian</b> , <a href="https://doi.org/10.1007/s00214-022-02932-3">https://doi.org/10.1007/s00214-022-02932-3</a>	2022
	32.5 nu e autor pp	8.948	Q1	<b>Energy &amp; Environmental Science</b> , High performance Li-, Na-, and K-ion storage in electrically conducting coordination polymers, Jiande Wang, Xiaolong Guo, Petru Apostol, Xuelian Liu, Koen Robeyns, Loïk Gence, <b>Cristian Morari</b> , Jean-François Gohy, Alexandru Vlad, <a href="https://doi.org/10.1039/D2EE00566B">https://doi.org/10.1039/D2EE00566B</a>	2022
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			Nowakowska, Rejaul Sk, S Fatemeh Mousavi, Mehdi Heydari, Meike Stöhr, Sameena S Zaman, <b>Cristian Morari</b> , Lutz H Gade, Thomas A Jung, <a href="https://doi.org/10.1021/acs.jpcelett.2c01592">https://doi.org/10.1021/acs.jpcelett.2c01592</a>	
15.1 nu e autor pp	3.548	Q1	<b>Advanced Science</b> , New Cathode Materials in the Fe-PO <sub>4</sub> -F Chemical Space for High-Performance Sodium-Ion Storage, Xuelian Liu, Jiande Wang, Mengyuan Du, Koen Robeyns, Yaroslav Filinchuk, Qi Zhu, Varun Kumar, Yann Garcia, <b>Gheorghe Borodi</b> , <b>Cristian Morari</b> , Jean-Francois Gohy, Alexandru Vlad, <a href="https://doi.org/10.1002/advs.202200924">https://doi.org/10.1002/advs.202200924</a>	2022
22 nu e autor pp	5.615	Q1	<b>ACS Energy Letters</b> , A High-Voltage Organic Framework for High-Performance Na- and K-Ion Batteries, Jiande Wang, Xuelian Liu, He Jia, Petru Apostol, Xiaolong Guo, Fabio Lucaccioni, Xiaozhe Zhang, Qi Zhu, <b>Cristian Morari</b> , Jean-François Gohy, Alexandru Vlad, <a href="https://doi.org/10.1021/acsenergylett.1c02571">https://doi.org/10.1021/acsenergylett.1c02571</a>	2022
41.2 nu e autor pp	15.578	Q1	<b>Nature Materials</b> , Conjugated sulfonamides as a class of organic lithium-ion positive electrodes, Jiande Wang, Alae Eddine Lakraychi, Xuelian Liu, Louis Sieuw, <b>Cristian Morari</b> , Philippe Poizot, Alexandru Vlad, <a href="https://doi.org/10.1038/s41563-020-00869-1">https://doi.org/10.1038/s41563-020-00869-1</a>	2021
6.6 nu e autor pp	0.917	Q1	<b>Electrochimica Acta</b> , Optimized lead-acid grid architectures for automotive lead-acid batteries: An electrochemical analysis, Calborean, Adrian; Murariu, Teodora; <b>Morari, Cristian</b> , <a href="https://doi.org/10.1016/j.electacta.2021.137880">https://doi.org/10.1016/j.electacta.2021.137880</a>	2021
5.9 nu e autor pp	1.660	Q1	<b>Communications Chemistry</b> , Pyrazinacenes exhibit on-surface oxidation-state-dependent conformational and self-assembly behaviours, David Miklík, S Fatemeh Mousavi, Zuzana Burešová, Anna Middleton, Yoshitaka Matsushita, Jan Labuta, Aisha Ahsan, <b>Luiza Buimaga-Iarinca</b> , Paul A Karr, Filip Bureš, Gary J Richards, Pavel Švec, Toshiyuki Mori, Katsuhiko Ariga, Yutaka Wakayama, <b>Cristian Morari</b> , Francis D'Souza, Thomas A Jung, Jonathan P Hill, <a href="https://doi.org/10.1038/s42004-021-00470-w">https://doi.org/10.1038/s42004-021-00470-w</a>	2021
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			Jouhara, <b>Gheorghe Borodi, Cristian Morari, Philippe Poizot, Alexandru Vlad</b> , <a href="https://doi.org/10.1021/acs.chemmater.0c02989">https://doi.org/10.1021/acs.chemmater.0c02989</a>	
2.6	0.469	Q2	<b>Physics Letters A</b> , Weak interactions between tetraphenylporphyrin dimers: A Wannier orbitals study, Biter, Teodor-Lucian; <b>Buimaga-Iarinca, Luiza; Morari, Cristian</b> , <a href="https://doi.org/10.1016/j.physleta.2020.126717">https://doi.org/10.1016/j.physleta.2020.126717</a>	2020
		Q3		
9.4	1.169	Q1	<b>Journal of Energy Storage</b> , Resonance frequency analysis of lead-acid cells: An EIS approach to predict the state-of-health, Adrian Calborean, Olivia Bruj, Teodora Murariu, <b>Cristian Morari</b> , <a href="https://doi.org/10.1016/j.est.2019.101143">https://doi.org/10.1016/j.est.2019.101143</a>	2020
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3.7	0.469	Q2	<b>Physical Review B</b> , Topological superconductivity from magnetic impurities on monolayer NbSe <sub>2</sub> , Sticlet, Doru; <b>Morari, Cristian</b> , <a href="https://doi.org/10.1103/PhysRevB.100.075420">https://doi.org/10.1103/PhysRevB.100.075420</a>	2019
		nu e autor pp		
3.1	0.477	Q2	<b>Beilstein Journal of Nanotechnology</b> , The effect of translation on the binding energy for transition-metal porphyrines adsorbed on Ag(111) surface, <b>Buimaga-Iarinca, Luiza; Morari, Cristian</b> , <a href="https://doi.org/10.3762/bjnano.10.70">https://doi.org/10.3762/bjnano.10.70</a>	2019
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3.5	0.555	Q2	<b>Nanotechnology</b> , Charge transport pathways in metal porphyrin as interplay between long and short range scattering processes, <b>Buimaga-Iarinca, L.; Morari, C.</b> <a href="https://doi.org/10.1088/1361-6528/aaed75">https://doi.org/10.1088/1361-6528/aaed75</a>	2019
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		nu e autor pp		



## MINISTERUL CERCETĂRII, INOVĂRII ȘI DIGITALIZĂRII

Lista proiectelor de cercetare câștigate de candidat și valoarea acestora. (valoare >100.000 eu)

Project **PNCDI III - P4 - ID-PCE 2020-0824**, whose completion was evaluated as Excellent; Financed by UEFISCDI with 1200000 RON (approx. 240000 Euro); project duration: 36 months; project leader Dr. Cristian Morari

Project **PN-III-P4-ID-PCE-2016-0217** whose completion was evaluated as A+; Financed by UEFISCDI with 850000 RON (approx. 210000 Euro); project duration: 30 months; project leader Dr. Cristian Morari

Project **PN-II-PT-PCCA-2013-4-1226**. Over 40 researchers involved. Financed by UEFISCDI with 1250000 RON (approx. 310000 Euro); project duration: 39 months; project leader Dr. Cristian Morari

**ERANET-QUANTERA-2019-QuCos (2020 – 2024)** - Funded through Horizon2020, program P3-3.2 Horizon 2020-Quantera H2020. Total value is over 1400000 Euro (national and private funds) out of which Romanian Partner requested 122000 Eu; project leader Dr. Luiza Buimaga-Iarinca

Coordinator of 7 stages of **NUCLEU** project in INCDTIM during 2008-2023

To date, **the total amount of funds attracted or managed by Group** is approx. **1.700.000 euro**, from which approx. 920.000 euro represents competition research grants and approx. 770.000 euro came from intra-institutional grants (7 stages of **NUCLEU** program in INCDTIM between 2009-2023)



9. Lista brevetelor depuse și a celor acceptate, dacă este cazul.

**International patent request**

Derwent Primary Accession Number 2023-35756Q US2023107661-A1

<https://patents.google.com/patent/US20230107661A1/en>

Device for capturing free atoms or molecules or clusters or ions in quantum well structure, includes support layer of conductive or insulating material, conductive layer deposited on support layer and quantum well structure fabricated on conductive layer

Inventors MORARI I C; BUIMAGA-IARINCA L T; GADE L H; HEYDARI M; REJAUL S; AHSAN A; JUNG T

**Patents requested at the Romanian State Office for Inventions and Trademarks**

1. Derwent Primary Accession Number 2019-40690F, RO133009(A0)  
Method for determining life and quality of lead-acid batteries, involves tracking parameter of constant phase element with linear dependence on battery, slope of linear dependence of parameter and number of load cycles/discharge  
Inventors MORARI I C; BOT A; BUIMAGA-IARINCA L T; MURARIU A T
2. Derwent Primary Accession Number 2018-16004X, RO132400-A0  
METALLIC GRID WITH OPTIMIZED GEOMETRY FOR LEAD-ACID BATTERY POSITIVE ELECTRODE  
Inventors: BOT A; BUIMAGA-IARINCA L T; MORARI I C; MURARIU A T
3. Derwent Primary Accession Number 2018-16003Y, RO132401-A0  
METALLIC GRID FOR POSITIVE ELECTRODES IN ACID-LEAD BATTERIES, OPTIMIZED TO MINIMIZE MATERIAL CONSUMPTION IN MANUFACTURING PROCESS  
Inventors BOT A; BUIMAGA-IARINCA L T; MORARI I C; MURARIU A T
4. Derwent Primary Accession Number 2017-47386J, RO132016-A0  
INERT-MEDIUM ENCLOSURE FOR DIAGNOSING AND OPTIMIZING ACCUMULATOR ELECTRODE-GRIDS  
Inventors BOT A; MORARI I C; TUDORAN C



5. Derwent Primary Accession Number 2017-27305Q, RO131817-A2  
DEVICE AND PROCESS FOR DETERMINING CURRENT DISTRIBUTION IN  
ELECTRODE GRIDS OF ELECTROCHEMICAL POWER SOURCES  
Inventors TUDORAN C; MORARI I C; STREZA M
6. Derwent Primary Accession Number 2020-86770G RO134413(A0)  
Analysis method for determining life span of lead-acid battery, involves spending battery when  
resonant frequency that is doubled in relation to resonant frequency registered during first part  
of life span  
Inventors CALBOREAN A; MORARI I C

\* Se redactează în limba engleză. Prin excepție, redactarea cererii de premieră se face în limba română pentru cererile din domenii cu specific românesc: limba și literatura română și dreptul românesc.

\*\* Rezultatele activității de cercetare sunt evaluate conform Anexei nr. 3 la Regulamentul de organizare și funcționare a programului Gala Cercetării Românești.