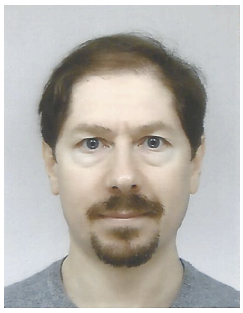
CURRICULUM VITAE

PERSONAL INFORMATION

Sergiu Arapan



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sergiu.arapan@gmail.com

Sex male | Date of birth 27/11/1973 | Nationality Romania, Moldova

WORK EXPERIENCE

from 01/04/2016

Senior postdoctoral researcher

International Center in Critical Raw Matreials (ICCRAM), University of Burgos, Spain

Applying structure predicting methods for the discovery and design of new Rare Earth free permanent magnetic materials within the EU-H2020-NMP23-NOVAMAG-GA-686056 project
Applying non-collinear spin-orbit coupling calculations to study the magneto-crystalline anisotropy of uniaxial magnetic structures
Developing classical force-fields to study the stability of grain-boundaries of magnetic materials and thermodynamic stability of magnetic compounds.

from 10/05/2011 – to 31/03/2015

Postdoctoral researcher

National Institute for Materials Science (NIMS), Tsukuba, Japan

Applying linear scaling DFT methods to study atomic level properties of SiGe nanostructures (quantum dots and quantum wires systems)
Performing molecular dynamics simulations with reactive force-field to simulate the oxidation of Si nanowires

from 01/01/2010 – to 30/04/2011

Postdoctoral researcher

Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Sweden

Applying DFT+U and hybrid functional methods for studying the formation of O vacancies and electronic charge localization effects in reduced ceria

from 01/11/2008 – to 31/12/2009

Postdoctoral researcher

Applied Material Division, Department of Material Science and Engineering, Royal Institute of Technology in Stockholm, Sweden

Applying ab-initio thermodynamics and phonon calculations for studying dynamical stability under high pressure and temperature conditions of Fe phases at the Earth interior and MgO in the Earth muntle.

from 1999 – to 2002

Researcher

Institute of Applied Physics, Academy of Sciences of Moldova, Chișinău, Republic of Moldova

Studying quantum size effects in semiconductor heterostructures

from 01/09/2000– to 31/05/2001

Lecturer

Free International University of Moldova, Chișinău, Republic of Moldova

Delivering lectures (in English) on general physics to foreign students

EDUCATION AND TRAINING

from 01/09/2002 – to 30/10/2008

Philosophy Degree in Physics

Materials Theory, Department of Physics and Astronomy, Uppsala University, Sweden

- Electronic structure calculation methods
- Classical force-field computational methods
- Phonon calculations
- Ab-initio thermodynamics
- Phase transitions under applied pressure
- Temperature driven phase transitions

from 01/09/1991 – to 31/05/1996

Diploma in Physics

Faculty of Physics, Chair of Theoretical Physics, Moldova State University, Republic of Moldova

- Theoretical methods based on model Hamiltonians
- Electronic states at the interface in semiconductor heterojunctions and quantum well structures

PERSONAL SKILLS

Mother tongue(s): Romanian, Russian

Other language(s)

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken interaction	Spoken production	
English	C1	C2	C1	C2	C1
French	B1	B1	B1	B1	B1
Spanish	B1	B1	A2	A2	A2
Swedish	A2	A2	A1	A1	A1
Japanese	A1	A1	A1	A1	A1

Replace with name of language certificate. Enter level if known.

Levels: A1/A2: Basic user - B1/B2: Independent user - C1/C2 Proficient user
Common European Framework of Reference for Languages

Communication skills

- good communication skills gained through my experience of working in various international research teams

Organisational / managerial skills

- leadership (co-supervising a PhD student and leading a small group)

Digital competence

	SELF-ASSESSMENT			
Information processing	Communication	Content creation	Safety	Problem solving
Independent user	Independent user	Independent user	Independent user	Independent user

Levels: Basic user - Independent user - Proficient user
Digital competences - Self-assessment grid

Replace with name of ICT-certificate(s)

- good programming skills in Fortran, C, Python, Mathematica
- good knowledge of Unix/Linux and Mac OS
- experience of administrating small computational clusters

Other skills: cooking

Publications

(h-index 9)

- P. Nieves, S. Arapan, T. Shrefl, and S. Cuesta-López, *Atomistic spin dynamics simulations of the MnAl τ-phase and its antiphase boundary*, Phys. Rev. B **96**, 224411 (2017).
- P. Nieves, S. Arapan, and S. Cuesta-López, *Exploring the crystal structure space of $CoFe_2P$ by using adaptive genetic algorithm methods*, IEEE Transaction on Magnetics **53**, 1 (2017).
- P. Nieves, S. Arapan, and S. Cuesta-López, *An adaptive genetic algorithm approach for predicting magnetic structures suitable for high-performance permanent magnet development*, Magnetic Conference INTERMAG, IEEE International 1-1 (2017).
- P. Nieves, S. Arapan, G. C. Hadjipanayis, D. Narchos, J. M. Barandiaran, and S. Cuesta-López, *Applying high-throughput computational techniques for discovering next-generation of permanent magnets*, Phys. Stat. Sol. (c), **13**, 942 (2016). DOI: 10.1002/pssc.201600103
- Sergiu Arapan, David R. Bowler, and Tsuyoshi Miyazaki, *A linear scaling DFT study of the growth of a new {105} facet layer on a Ge hut cluster,* (2015) http://arxiv.org/abs/1510.00526
- Sergiu Arapan, Sergei I. Simak, and Natalia V. Skorodumova, *Volume-dependent electron localization in ceria,* Phys. Rev. B. **91**, 125108 (2015). http://dx.doi.org/10.1103/PhysRevB.91.125108
- S. Arapan, D. Bowler, and T. Miyazaki, *A first-principle study of adsorption of Ge dimers on Ge hut cluster by linear scaling DFT methods*, 日本物理学会講演概要集 **69**, 870 (2014).
- Michiaki Arita, Sergiu Arapan, David R. Bowler, and Tsuyoshi Miyazaki, *Large scale DFT simulations with a linear-scaling DFT code Conquest on K-computer,* J. Adv. Simulat. Eng. Sci. **1**, 87 (2014), doi:10.15748/jasse.1.87
- Chang Sun Kong, Wei Luo, Sergiu Arapan, Pierre Villars, Shuichi Iwata, Rajeev Ahuja, and Krishna Rajan, *Information-Theoretic Approach for the Discovery of Design Rules for Crystal Chemistry*, J. Chem. Inf. Model. **52**, 1812 (2012).
- P. Souvatzis, S. Arapan, O. Eriksson, and M. I. Katsnelson, *Temperature-driven α-to-β phase transformation in Ti, Zr and Hf from first-principles theory combined with lattice dynamics,* EuroPhys. Lett. **96**, 66006 (2011). http://dx.doi.org/10.1209/0295-5075/96/66006
- A. B. Belonoshko, S. Arapan, and A. Rosengren, *An ab initio molecular dynamics study of iron phases at high pressure and temperature,* J. Phys.: Condens. Matter **23**, 485402, (2011). http://dx.doi.org/10.1088/0953-8984/23/48/485402
- Sergiu Arapan and Rajeev Ahuja, *High-pressure phase transformations in carbonates,* Phys. Rev. B **82**, 184115 (2010). http://dx.doi.org/10.1103/PhysRevB.82.184115
- A. B. Belonoshko, S. Arapan, R. Martonak, and A. Rosengren, *MgO phase diagram from first principles in a wide pressure-temperature range,* Phys. Rev. B **81**, 054110 (2010). http://dx.doi.org/10.1103/PhysRevB.81.054110
- Wei Luo, Börje Johansson, Olle Eriksson, Sergiu Arapan, Petros Souvatzis, Mikhail I. Katsnelson, and Rajeev Ahuja , *Dynamical stability of body center cubic iron at the Earth's core conditions*, Proc. Natl. Acad. Sci. USA **107,** 9962 (2010). doi:10.1073/pnas.1004076107
- Sergiu Arapan, Natalia V. Skorodumova, and Rajeev Ahuja, *Determination of the Structural Parameters of an Incommensurate Phase from First Principles: The Case of Sc-II,* Phys. Rev. Lett. **103**, 085701 (2009). http://dx.doi.org/10.1103/PhysRevLett.102.085701
- Anders Modin, K. O. Kvashnina, S. M. Butorin, Lars Werme, Joseph Nordgren, Sergiu Arapan, Rajeev Ahuja, A. Fallberg, Mikael Ottosson, *Electronic structure of Cu_3N films studied by soft x-ray spectroscopy*, J. Phys.: Condensed Matter **20**, 235212 (2008).
- Sergiu Arapan, Ho-kwang Mao, and Rajeev Ahuja, *Prediction of incommensurate crystal structure in Ca at high pressure,* Proc. Natl. Acad. Sci. USA **105**, 20627 (2008). doi:10.1073/pnas.0810813105
- Sergiu Arapan, *Understanding Physical Reality via Virtual Experiments*, Acta Universitatis Uppsaliensis (2008). http://www.diva-portal.org/smash/get/diva2:172636/FULLTEXT01.pdf
- Sergiu Arapan, Jailton Souza de Almeida, and Rajeev Ahuja, *Formation of sp^3 Hybridized Bonds and Stability of $CaCO_3$ at Very High Pressure,* Phys. Rev. Lett. **98**, 268501 (2007). http://dx.doi.org/10.1103/PhysRevLett.98.268501
- S. C. Arapan, M. A. Liberman, *Exciton levels and optical absorption in coupled double quantum well structures,* J. Lumin. **112**, 216, (2005). http://dx.doi.org/10.1016/j.jlumin.2004.09.059
- S. C. Arapan, S. V. Korepov, M. A. Liberman, and B. Johansson, *Effect of the boundary roughness on the conductance of double quantum wire in a magnetic field,* EuroPhys. Lett. **64**, 239 (2003). http://dx.doi.org/10.1209/epl/i2003-00313-4
- S. C. Arapan, S. V. Korepov, M. A. Liberman, and B. Johansson, *Conductance of a disordered double quantum wire in a magnetic field: Boundary roughness scattering*, Phys. Rev. B **67**, 115328 (2003). http://dx.doi.org/10.1103/PhysRevB.67.115328

Projects

NOVAMAG: NOVel, critical materials free, high Anisotropy phases for permanent MAGnets, by design. EU-HORIZON2020-686065

Scientific & Technical Reports

- P. Nieves, S. Arapan, T. Shrefl, H. C. Herper, and S. Cuesta-López, *Report on temperature dependence of the intrinsic magnetic properties properties of MnAl*, NOVAMAG Deliverable D4.3 (2017).
- H. C. Herper, O. Vekilova, O. Eriksson, S. Arapan, P. Nieves, S. Cuesta-López, H. Zhang, J. Gassmann, *Final report on preselected sets of structural optimized candidate phases for novel PM of the type* $(Fe,Co)_{100-x-y}M_x(X1)_y$, $RFe_{12-x}(X5)_x$, *FeNi(X2), FeCo(X3) and MnAl(X4)*, NOVAMAG Deliverable 1.8 (2017).
- S. Arapan, P. Nieves, C. Pecoraro, S. Cuesta-López, and T. Schrefl, *Final report on the simulated effect of structural disorder at grain boundaries or surfaces*, NOVAMAG Deliverable 4.2 (2017).
- S. Arapan, C. Pecoraro, P. Nieves, S. Cuesta-López, *Development of DFT-based classical potentials for molecular dynamics simulations,* NOVAMAG Deliverable 1.7 (2017).
- S. Arapan, P. Nieves, S. Cuesta-López, T. Schrefl, and M. Sgroi, *1st report on the simulated effect of structural disorder at grain boundaries or surfaces*, NOVAMAG Deliverable 4.1 (2017).
- H. C. Herper, O. Vekilova, O. Eriksson, S. Arapan, P. Nieves, and S. Cuesta-López, *Report on exchange parameters for the identified phases for spin dynamics studies*, NOVAMAG Deliverable D2.3 (2017).
- H. C. Herper, O. Vekilova, O. Eriksson, S. Arapan, P. Nieves, and S. Cuesta-López, *Report on the Curie temperature and magnetization for optimized structures of the most promising phases*, NOVAMAG Deliverable D2.2 (2017).
- H. C. Herper, O. Vekilova, O. Eriksson, S. Arapan, P. Nieves, and S. Cuesta-López, *Report on the anisotropy data for the identified phases*, NOVAMAG Deliverable D2.1 (2017).
- S. Arapan, C. Pecoraro, P. Nieves, S. Cuesta-López, *1st report on the development of DFT-based classical potentials for molecular dynamics simulations,* NOVAMAG Deliverable 1.6 (2017).
- S. Arapan, P. Nieves, and S. Cuesta-López, *Report on the implementation and validation of the AGA for the stabilization of non-cubic structures in FeNi, FeCo, MnAl and Fe-based RE lean systems* RFe_{12}, NOVAMAG Deliverable D1.5 (2017).
- P. Nieves, S. Arapan, and S. Cuesta-López, *1st report on the implementation and validation of the AGA for the stabilization of non-cubic structures in FeNi, FeCo, MnAl and Fe-based RE lean systems* RFe_{12}, NOVAMAG Deliverable D1.4 (2016).
- P. Nieves, S. Arapan, and S. Cuesta-López, *Report on the implementation and validation of the AGA for the* $(Fe,Co)_{100-x-y}M_x(X1)_y$ *systems,* NOVAMAG Deliverable D1.3 (2016).
- P. Nieves, S. Arapan, and S. Cuesta-López, *1st report on the implementation and validation of the AGA for the* $(Fe,Co)_{100-x-y}M_x(X1)_y$ *systems,* NOVAMAG Deliverable D1.2 (2016).
- P. Nieves, S. Arapan, H. C. Herper, S. Cuesta-López, T.Srefl, and H. Zhang, *Complete MODA tables describing all simulations to be carried out in NOVAMAG,* NOVAMAG Deliverable D1.1 (2016).

Conferences & workshops

- P. Nieves, S. Arapan, M. A. Cerderia, R. Iglesias, and S. Cuesta-López, *Critical raw material problem in high-performance permanent magnets under extreme conditions*, E-MRS, Warsaw, Poland (2017).
- C. Pecoraro S. Arapan, P. Nieves, S. Cuesta-López, *Developing classical force-field potentials for the massive exploration of new permanent magnets without critical raw materials*, , E-MRS, Warsaw, Poland (2017).
- P. Nieves, S. Arapan, and S. Cuesta-López, *An Adaptive Genetic Algorithm approach for predicting magnetic structures suitable for high-performance permanent magnet development,* INTERMAG-2017, Dublin, Ireland (2017).
- S. Arapan, P. Nieves, and S. Cuesta-López, *Predicting magnetic structures by usin adaptive genetic algorithms and DFT calculations,* CONQUEST Workshop, Bordeaux, France (2017).
- R. Barros, R. Serrano-López, L. Romero-Santacreu, P. Nieves, S. Arapan, M. Perez-Cabo, and S. Cuesta-López, *Sustainable design of materials for high exigency industry using complementary capabilities and circular economy strategies*, International Industrial Workshop, Burgos, Spain (2017).
- P. Nieves, S. Arapan, and S. Cuesta-López, *The Adaptive Genetic Algorithm for predicting structures suitable for the next-generation of permanent magnets*, 10th RES users Conference, León, Spain (2016).
- R. Barros, R. Serrano-López, L. Romero-Santacreu, P. Nieves, S. Arapan, and S. Cuesta-López, *Unique methodology to develop innovative materials for extreme application using complementary capabilities: multiscale modelling, critical raw materials substitution, eco-design and nanosafety assessment,* Industrial Technologies Congress, Amsterdam, Holland (2016).
- S. Arapan, D. Bowler, and T. Miyazaki, *A first principle study of the adsorption of Ge dimers on Ge hut clusters by linear scaling DFT methods,* JPS meeting, Tokyo, Japan (2014).
- S. Arapan, D. Bowler, and T. Miyazaki, *First principle simulations of Ge dimers adsorption on the {105} facets of a Ge hut cluster,* JSST Conference, Tokyo, Japan (2013).
- S. Arapan, D. Bowler, and T. Miyazaki, *Ab initio study of the nucleation of Ge dimers on the {105} facets of a Ge hut*, 16th International Workshop on Computational Physics and Material Science: Total Energy and Force Methods, Trieste, Italy (2013).
- A. Belonoshko, S. Arapan, L. Koci, and A. Rosengren, *Mechanism of body-centered cubic phase stabilization of Fe and He at high pressure and temperature*, APS Meeting, USA (2012).
- S. Hahn, S. Arapan, B. Harmon, and O. Eriksson, *Calculated temperature dependence of elastic constants and phonon dispersion of hcp and bcc beryllium*, APS Meetings (2011).
- T. Kubart, S. Arapan, N. V. Skorodumova, T. Nyberg, and S. Berg, *Molecular dynamics simulations of low energy Ar sputtering of TiO_2 surface*, Proceedings of the 9th International Conference on Reactive Sputter Deposition, Ghent, Belgium (2010).
- S. Arapan, and R. Ahuja, *High-pressure phase transformations in aragonite, strontianite and witherite,* Crystallographic Congress IUCr 2008, Osaka, Japan (2008).

ANNEXES