

RAZVAN CARACAS
CURRICULUM VITAE
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PERSONAL INFORMATION

Researcher unique identifier(s) (Research ID): C-8115-2012

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Current professional address:

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• **EDUCATION**

- 2010 **HdR** (Habilitation à Diriger des Recherches) “Earth and planetary materials from a computational perspective”, Ecole Normale Supérieure de Lyon, Lyon, France
- 2003 **Ph.D.** (Material Physics) “First-principles study of materials involved in incommensurate transitions”, Université Catholique de Louvain, Louvain-la-Neuve, Belgium
- 2002 **M.Sc.** (Material Physics) “Ab initio simulations of incommensurate phases” Université Catholique de Louvain, Louvain-la-Neuve, Belgium
- 1997 **B.Sc.** (Geology and Geophysics), “Structural morphology of crystals. Application to oxide minerals”, Universitatea Bucuresti, Bucharest, Romania

• **EMPLOYMENT**

- 2014 – Directeur de Recherche (Senior Researcher), Centre National de la Recherche Scientifique, Laboratoire de Géologie de Lyon, Lyon, France
- 2007 – 2014 **Chargé de Recherche**, CNRS, Laboratoire de Géologie de Lyon, Lyon, France
- 2007 – 2008 **Humboldt FelloW**, Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany
- 2006 – 2007 **Post-doctoral/Research associate**, Bayerisches Geoinstitut, University of Bayreuth, Bayreuth, Germany
- 2004 – 2006 **Carnegie Fellow**, Carnegie Institution of Washington, Geophysical Laboratory, Washington, DC, USA
- 2003 – 2004 **Post-doctoral/Research associate**, Univ. of Minnesota, Dept. Chem. Engineering and Materials Sci., Minneapolis, MN, USA
- 1997 – 2003 **Teaching assistant**, Université Catholique de Louvain, Faculty of Sciences, Louvain-la-Neuve, Belgium
- 1995 – 1997 **Research assistant**, Universitatea Bucuresti, Faculty of Geology and Geophysics, Mineralogy Dept., Bucharest, Romania
- 2007 – 2010 **Visiting scientist**, Carnegie Institution of Washington, Geophysical Laboratory, Washington, DC, USA

- **FELLOWSHIPS AND AWARDS**

- 2015 European Research Council Consolidator Grant: “IMPACT. The giant impact and the Earth and Moon formation”
- 2013 Research Excellence Medal of the European Mineralogical Union
- 2013 Prime d’Excellence Scientifique, CNRS, France
- 2012 Prix Henri Buttgenbach, Academie Royale des sciences, des letters et des beaux-arts de Belgique, Bruxelles, Belgium
- 2008: Poster Prize, ScSSI (Science of the Solar System Ices) Workshop
- 2007 – 2008 Humboldt Fellowship, Bayerisches Geoinstitut, University of Bayreuth, Germany
- 2004 – 2006 Carnegie Postdoctoral Fellowship, Geophysical Laboratory, Carnegie Institution of Washington, USA
- 1995 1st award Robert Weimar in Sedimentology, University of Bucharest, Romania
- 2012 Outstanding Student Paper Awards - Mineral and Rock Physics (MRP) awarded to Aaron S. Wolf, Caltech, for a presentaion on "Thermodynamic phase relations in the MgO-FeO-SiO₂ system in the lower mantle". Co-authoring: R. Caracas, P. Asimow.

- **SCIENTIFIC PRODUCTION**

- 67 peer-reviewed articles with a total of 5600+ citations, 21 *h*-index (acc. to Google Scholar), 41 *i*-10 index (acc. to Google Scholar)
- 8 conference proceedings
- 6 book chapters
- 159 oral presentations (out of which 67 invited)

- **PATENTS**

- Ordered Oxynitride Perovskites – Inventors: Ronald E. Cohen and Razvan Caracas
 - US Patent 8,287,831(2012);
 - US Patent 20,130,071,312 (2013);
 - Korea Patent 10-1489849 (2015).

- **RESEARCH GRANTS**

- Financial (PI-only listed)
- 2016 – 2021 “IMPACT: The Giant Impact and the Earth and Moon Formation”, ERC Consolidator Grant, **1.9 Million Euros**
- 2016 “Realistic geological melts during the giant impact: thermodynamics and possible remote identification”, CNRS INSU support grant, **5 kEuros**
- 2013 – 2017 “Carbonatite melts in the Earth’ mantle”, **40 kUSD**, Deep Carbon Observatory Support Grant of the Extreme Physics and Chesmitry Directorate
- 2012 – 2015 “Minor element partitioning between metal and silicate melts during core formation”, **100 kEuros**, PhD scholarship from the French Ministry of

Education

- 2013 - 2015 “Carbonated fluids and melts of the Earth’s mantle” CNRS PICS Cooperation grant for travel to Carnegie Institution – **18 kEuros**
- 2013 – 2014 “Element partitioning in the magma ocean” PROCOPE - French-German travel grant, **12 kEuros**
- 2010 – 2014 “The light elements of the Earth's core” CIBLE project with the Rhone-Alpes region, **118 kEuros** (including PhD scholarship)
- 2010 – 2013 “The light elements of the Earth's core”, CNRS INSU support grants, **24 kEuros**
- 2010 – 2011 “Multidisciplinary studies of structures in the deep mantle”, PROCOPE - French-German travel grant, **12 kEuros**
- 2008 – 2009 “Iron distribution in the Earth's mantle”, CNRS INSU support grants, **22 kEuros**
- 2007 – “WURM - a database of computed Raman spectra for minerals”, Private funding of **450 kEuros**, 2007-present.

Computational (in CPU hours)

“Mineralogy of the deep Earth from a computational perspective”
(DARI Grant x201X106368)

- 2016 3,200,000 CPU hours on CURIE @ CCRT
2,700,000 CPU hours on IBM @ IDRIS
3,900,000 CPU hours on SGI @ CINES
- 2015 2,650,000 CPU hours on CURIE @ CCRT
2,240,000 CPU hours on IBM @ IDRIS
6,420,000 CPU hours on SGI @ CINES
- 2014 1,200,000 CPU hours on CURIE @ CCRT
250,000 CPU hours on IBM @ IDRIS
2,340,000 CPU hours on SGI @ CINES
- 2013 1,400,000 CPU hours on CURIE @ CCRT,
1,900,000 CPU hours on SGI @ CINES
- 2012 1,900,000 CPU hours on SGI @ CINES
- 2011 1,800,000 CPU hours on SGI @ CINES
- 2010 100,000 CPU hours on Bull Itanium @ CCRT,
1,800,000 CPU hours on SGI @ CINES
- 2009 “Computational study of Earth and planetary materials,
80,000 CPU hours on IBM @ IDRIS,
570,000 CPU hours on SGI @ CINES
- 2009 “Planetary ices and molecular crystals under extreme conditions”
100,000 CPU hours on IBM @ IDRIS,
120,000 CPU hours on SGI @ CINES
- 2008 “Planetary materials: high-density C-O-N-H fluids”, BSC grants FI-2008-1-0015
and FI-2008-2-0027,
770,000 CPU on Caesar Augusta, University of Zaragoza, National Center of
Supercomputing, Spain.
- 2005 – 2013 (Co-PI) “Computational study of Earth and planetary materials”, NSF
grant MCA07S009,
~ 1 million CPU hours on a series of supercomputers on Teragrid

- **SUPERVISION OF STUDENTS AND RESEARCHERS**

- Researchers:

- * Ema Bobocioiu, *Raman spectra of the WURM project*, since 2008

- PhD students:

- * Jean-Alexis Hernandez, *First-principles modeling of the superionic phases and of the rheology of dense water ices under extreme conditions of pressure and temperature*, will defend in 2018

- * Alexandra Catalina Seclaman, *Chemical and physical behavior of trace elements in the silicate melts of the Earth's mantle*, graduating april 2016

- * Alexandre Martin, *Calculations of the linear response under strain and electric field in the Projector Augmented Wave formalism. Application to the computation of the sound wave velocities for relevant materials in geophysics*, graduated fall 2015 (co-supervised with Marc Torrent, CEA)

- * Baptiste Journaux, *Mineralogical study of planetary ices under pressure*, graduated in 2013 (co-supervised with Isabelle Daniel)

- * Lucile Bezacier, *Elastic properties of hydrated minerals: Application to the seismic anisotropy in the subduction zones*, graduated in 2011 (co-supervised with Bruno Reynard)

- Master students:

- * Nina Bothamy, *Raman spectra of Na-based Martian sulfates*, graduated in 2015

- * Eugenia Vasile, *Raman spectra in the magnesite – dolomite – calcite series*, graduated in 2014

- * Alina Ilie, *Raman spectra diamond and related phases at high temperature*, graduated in 2014

- * Vincent Clesi, *Elasticity of Fe³⁺-bearing perovskite and post-perovskite*, graduated in 2012

- * Christian Cardenas, *Mineral interfaces in the lower mantle*, graduated in 2012

- * Alejandra Vargas Calderon, *Fe₃C under pressure*, graduated in 2010

- * Rosa Davila Martinez, *Methanol monohydrate under pressure*, graduated in 2010

- BSc. students:

- * Olivier Hercot, graduated in 2002 (co-supervisor Prof. Jean Naud, Université Catholique de Louvain)

- * Colinne Lannoye, graduated in 2003 (co-supervisor Prof. Jean Naud, Université Catholique de Louvain)

- **TEACHING**

- At ENS Lyon (courses + practicals):

- 2009 – “Physics of Minerals I” class for Master 1 curriculum, ENS de Lyon

- 2009 – “Physics of Minerals II” class for Master 2 curriculum, ENS de Lyon

- 2007 – 2009 One module on computational mineralogy in the "Physics of the Earth" class from the Master curriculum

- At Université Catholique de Louvain (practicals)

- 2000 – 2003 Geological cartography (2nd year, Geology and Geography students)

- 2000 – 2001 Optics (2nd year, Geology students)

- 1998 – 2002 Introduction to Earth Sciences (1st year, students in the Faculty of Sciences and Faculty of Agronomical Sciences)

- 1998 – 2001 Thermodynamic geochemistry (3rd year, Geology students)

- 1998 – 2001 Ore mineralogy (4th year, Geology students)

1997 – 2001 Mineralogy (2nd year, Geology students)

• **ORGANISATION OF SCIENTIFIC MEETINGS**

- PI of the Proposal for bringing the International Mineralogical Association 2022 General Meeting to Lyon, France
- 2016 “Thermodynamic and ab initio modeling of natural fluids and melts” – CECAM international school; **Co-organizer**; Lausanne, Switzerland
- 2015 “Carbon at extreme conditions” – CECAM meeting, **Main PI**, Lugano, Switzerland
- 2014 “WURM Raman school” – CNRS school, **Director**, Lyon, 30 students
- 2014 “Dynamical, dielectric and magnetic properties of solids with ABINIT “ – CECAM international school; **Director**, Lyon, France; 28 students
- 2012 “Response treatment for the dynamical properties of materials with the ABINIT package” – CECAM international school; **Co-organizer**; Zürich, Switzerland; 40 students
- 2011 “Dynamical Properties of Earth and Planetary Materials” – CECAM international workshop; **Director**; Lausanne, Switzerland; 30 participants
- 2010 “Linear and non-linear responses of solids with the ABINIT software: phonons, electric fields, and other perturbations” – CECAM international school; **Co-organizer**; Lausanne, Switzerland; 40 students
- 2008 “The Science of Solar System Ices (ScSSI): A Cross-Disciplinary Workshop”; **Member** of the International Organizing Committee; 80 participants; Oxnard, California.
- 2005 – Main- or co-organizer of 30+ special sessions in international conferences

• **SOFTWARE DEVELOPMENT**

- 2001 MeandSym – C software used to create random meander channels “with different geostatistical constraints (unpublished)
- 1997 ATM2DXF – Visual Basic software used to create *.dxf files of mineral structures (published in the Proceedings vol. of the Romanian Conference on Advanced Materials, Bucharest, 1997).
- 1997 Madelung – Visual Basic software used to compute Madelung energies and electrostatic potentials for ionic crystals (published in Ann. Univ. Buc., Geology, 1998)
- 1996 FracDim – Matlab-based software used to measure fractal dimensions of 2D objects (unpublished)

ABINIT development

- implementation of the magnetic and non-magnetic symmetry space groups and related subjects (symmetrization of the stresses, the dynamical matrices, etc.)
- development of cut3d, a tool used to build 1-, 2- and 3-Dimensional sections through grid-like crystallographic objects (like electron density, potential, Fermi surface etc)
- implementation of the automatic construction of the maximally-localized lattice Wannier functions from the calculated phonon band structures (in collaboration

with Prof. Karin Rabe, Rutgers University of New Jersey, Dept. of Physics and Astrophysics)

- utility for automatic generation of the crystal structures of elements for tests of the pseudopotentials
- utility for automatic recognition of the symmetry labels for vibrational modes in Gamma
- various other crystallographic utilities, mainly dealing with the generation of the symmetry space groups and visualization of the symmetry operations.
- implementation of the response under strain and the automatic calculation of the elastic constants tensor within the framework of the planar augmented wavefunctions (co-PI)

• **FIELDTRIPS**

- 2000 – 2002 different short fieldtrips in the Paleozoic sedimentary regions of Southern Belgium mentoring 1st year undergraduate students in Geology (Université Catholique de Louvain)
- 1998 the sedimentary region of the Southern Pyrenees Mts.
- 1998 Massif des Maures (metamorphism) and Massif de l'Esterel (volcanism), S of France, mentoring 2nd year undergraduate students in Geology (Université Catholique de Louvain)
- 1997 – 2001 different short fieldtrips in the metamorphic regions of the Southern Carpathians
- 1997 Sokli carbonatite, Northern Finland, sampling for Nb ores

• **MULTIMEDIA TOOLS**

A 60 minutes videotape with computed crystal structures animations, realized using home-made software (e.g. ATM2SXF) and 3DStudio, presented in 1997, Bucharest.

• **MEDIA COVERAGE**

- 2016 Radio show “Planet – The world in which we will leave” at the Romanian Cultural Radio, Bucharest, Romania, about the ERC Consolidator Grant
- 2013 Press release of the INSU, CNRS about the 2013 Research Excellence Medal of the European Mineralogical Union
- 2006 “You don’t understand the pressure” by J. William Bell, in Acces, 19 (3), 7-10, published by the National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign

• **COMMISSIONS OF TRUST**

- 2010 – Editorial Board @ European Journal of Mineralogy
- 2014 – Editorial Board @ Earth and Planetary Materials, Frontiers in Astronomy and Space Sciences, Earth Science and Materials
- 2013 – 2016 Member of C4 (Comité des Chercheurs Calculant au CINES – French supercomputing center), Ministry of Research, France

- 2010 – Chair of the Theoretical and computing mineral physics sub-commission of the Physics of Minerals commission of the International Mineralogical Association.
- 2010 – 2012 Editorial Board @ Earth, Moon Planets, Elsevier
- 2009 – 2011 Member of the AGU Program Committee, on behalf of the MRP Focus Group
- 2009 – Member of the Mineral and Rock Physics Committee of the American Geophysical Union

• **INSTITUTIONAL RESPONSIBILITIES**

- 2016 – Council Board, Laboratoire de Géologie de Lyon, Lyon, France
- 2014 – Scientific Advisory Board, Observatoire des Sciences de l'Univers (OSU) Lyon, Université Claude-Bernard Lyon 1, Lyon, France
- 2012 – 2014 Organizer of the Internal Seminar Series, Laboratoire de Géologie de Lyon, ENS Lyon

• **MEMBERSHIPS OF SCIENTIFIC SOCIETIES**

- 2012 – Member, European Association of Geochemistry
- 2011 – Member, European Geophysical Union
- 2004 – Member, American Geophysical Union
- 2005 – Member, American Mineralogical Society

• **LANGUAGES**

- Romanian Native
- English Fluent
- French Fluent
- German Intermediate
- Italian Intermediate