

CURRICULUM VITAE

RAZVAN CARACAS

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PERSONAL INFORMATION

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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, Ecole Normale Supérieure de Lyon, Lyon, France
- 2018 – **Adjunct professor**
Centre for Earth Evolution and Dynamics, University of Oslo, Oslo, Norway

- 2007 – 2014 **Chargé de Recherche**, CNRS, Laboratoire de Géologie de Lyon, Ecole Normale Supérieure 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**, University of Minnesota, Department of Chemical Engineering and Materials Science, Minneapolis, MN, USA
- 1997 – 2003 **Teaching assistant**, Université Catholique de Louvain, Faculty of Sciences, Louvain-la-Neuve, Belgium
- 1995 – 1997 **Research assistant**, University of Bucharest, Faculty of Geology and Geophysics, Department of Mineralogy, Bucharest, Romania
- 2007 – 2010 **Visiting scientist**, Carnegie Institution of Washington, Geophysical Laboratory, Washington, DC, USA

- **FELLOWSHIPS AND AWARDS**

- 2016 Ad Astra Award for Excellence in Research, Earth and Space Sciences
- 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 lettres 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 presentation on "Thermodynamic phase relations in the MgO-FeO-SiO₂ system in the lower mantle". Co-authoring: R. Caracas, P. Asimow.

- **SCIENTIFIC PRODUCTION**

- 96 peer-reviewed papers with a total of 8900+ citations, 30 *h*-index, 61 *i*-10 index (acc. to Google Scholar); 6100+ citations, 25 *h*-index (acc. to Web of Science)
- 198 oral presentations (out of which 85 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**
- 2017 – 2019 “Carbon-bearing silicate melts” **30 kUSD**, Deep Carbon Observatory Support Grant of the Extreme Physics and Chemistry Directorate
- 2016 “Realistic geological melts during the giant impact: thermodynamics and possible remote identification”, CNRS INSU support grant, **5 kEuros**
- 2016 – 2018 “Stability of carbonate minerals and the carbon hosts in the Earth’s deep mantle” CNRS PICS Cooperation grant for travel to Caltech – **18 kEuros**
- 2013 – 2017 “Carbonatite melts in the Earth’ mantle”, **40 kUSD**, Deep Carbon Observatory Support Grant of the Extreme Physics and Chemistry 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 – 2016 “WURM - a database of computed Raman spectra for minerals”, Private funding of **450 kEuros**.

Computational (in CPU hours)

Sources:

DARI Grant x201X106368, France

PRACE grant

NOTUR Norwegian grant

Amounts

- 2020 5,000,000 CPU hours on Jean-Zay @ IDRIS
30,000,000 CPU hours on a PRACE grant on Irene-AMD @ CCRT
5,000,000 CPU hours on Fram at Univett/Sigma2
- 2019 22,402,560 CPU hours on OCCIGEN @ CINES
4,000,000 CPU hours on ADA @ IDRIS
7,000,000 CPU hours on IRENE KNL @ CCRT

2018 16,378,908 CPU hours on OCCIGEN @ CINES
4,385,357 CPU hours on ADA @ IDRIS
2,681,972 CPU hours on CURIE @ CCRT

2017 6,464,000 CPU hours on CURIE @ CCRT
4,339,000 CPU hours on IBM @ IDRIS
11,080,000 CPU hours on SGI @ CINES

2016 3,700,000 CPU hours on CURIE @ CCRT
2,970,000 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**

Current:

Post-doctoral researchers:

* Dr. Natalia Solomatova, *Volatiles-bearing silicate melts during the Giant Impact*, IMPACT project, October 2017 –

* Dr. Mandy Bethkenhagen, *Silicate melts during the Giant Impact*, IMPACT project, January 2020 –

Researchers:

* Dr. Ema Bobocioiu, *Raman spectra of the WURM project*, since 2008; *Electronic and vibrational properties of silicate glasses*, IMPACT since 2016

PhD students:

- * Tim Bögels, *Behavior of major rock-forming minerals during the Giant Impact*, IMPACT project, starting November 2019
- * Renata Brandelli Schaan, *Behavior of volatiles during the Giant Impact*, IMPACT project, starting November 2018
- * Anais Kobsch, *Supercritical silicate melts*, IMPACT project, starting September 2017
- * Zhi Li, *Fe-based alloys during the Giant Impact*, IMPACT project, starting October 2017

Former:

Post-doctoral researchers:

- * Dr. Francois Soubiran, ABISSE – *Ab initio simulations for Super-Earths*, Marie-Curie Fellow, starting September 2017 – August 2019

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*, graduated July 2017
- * Alexandra Catalina Seclaman, *Chemical and physical behavior of trace elements in the silicate melts of the Earth's mantle*, graduated 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 October 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:

- * Anais Kobsch, *Supercritical state in the feldspars mineral system*, graduated in 2017
- * 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:

- * Helene Plihon, graduated in 2018
- * 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 + labs):

- 2009 – “Physics of Minerals I” class for Master 1 curriculum, ENS de Lyon (3 credits, 30 hours)
- 2009 – “Physics of Minerals II” class for Master 2 curriculum, ENS de Lyon (3 credits, 30 hours)
- 2007 – 2009 One module on computational mineralogy in the "Physics of the Earth" class from the Master curriculum
At Université Catholique de Louvain (labs)
- 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**

- 2022 President of the 23rd General Meeting of the International Mineralogical Association 2022, Lyon, France
- 2021 “Empirical and ab initio thermodynamic models of minerals and melts” – **Co-organizer**
Villefranche-sur-Mer, France, expected about 40 students
- 2020 “WURM Raman school” – **Organizer**
Lyon, France, 40 students
- 2020 “Empirical and ab initio thermodynamic models of minerals and melts” – **Co-organizer**
Milos, Grece, expected about 40 students
- 2017 “Ab initio tools for hypothesis testing” – **Co-organizer**;
Compres 2017, pre-meeting workshop/school, Tamaya Resort, New Mexico, USA, 25 participants
- 2017 “ABIDEV 2017: The 8th ABINIT developers workshop” – **Co-organizer**;
Fréjus, France, 40 participants
- 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 a large number of special sessions in international
conferences

• SOFTWARE DEVELOPMENT

UMD package

The Universal Molecular Dynamics package is a python-based open-source package to analyze the results stemming from ab initio molecular-dynamics simulations of fluids. The package allows the computation of a series of structural, transport and thermodynamic properties.

ABINIT development (1998 – 2003)

- 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)

- 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)

- **OUTREACH: exhibition**

MOON IMPACT – a geological story

On May 16th, 2020 we will launch the itinerant international exhibition “Moon Impact – a geological story” at the National Museum of Geology of Romania, in Bucarest. Over almost 220 square meters of exhibition you will be able to learn about the formation of the solar system, about the Giant Impact that generated the protolunar synestia, and about the ever-growing complexity of the mineral realm. You will admire distant proto-planetary disks, you will see animations of giant impacts and you will peek into the atomic secrets of the formation of the first atmosphere of the Earth.

The exhibition tells the story of the Giant impact and the Moon formation in the context of the geological evolution of the Earth and of the solar system. It covers five rooms dedicated to science, one planetarium, and one room dedicated to art and science.

The science rooms, in order, speak about:

1. Formation of the solar system, and other solar systems and planetary nebula
2. The Giant Impact, the formation of the Moon, and the early Earth.
3. The Moon today, similarities and differences between the Moon and the Earth, the conquest of space
4. A parallel between the mineral diversification and the life evolution
5. Anthropocene

- **MEDIA COVERAGE**

- | | |
|------|--|
| 2017 | A series of highlights related to the discovery of a new high-pressure form of cristobalite silica; in: Phys.org, DESY news, UPI.com, Science Daily |
| 2017 | A highlight on the GENCI (The French Group of Supercomputing Centers) website about the recent activity of the computational mineralogy group in Lyon. |
| 2016 | An article at the HotNews.ro news agency about the Ad Astra awards 2016, for the Award on Excellence in Research, Earth and Space Sciences |
| 2016 | An article in the Swiss weekly Le Matin Dimanche about the new Science paper on the role of pressure on Fe isotope partitioning and the content in light elements of the Earth’s core. |
| 2016 | Radio show “Planet – The world in which we will leave” at the Romanian Cultural Radio, Bucharest, Romania, about the ERC Consolidator Grant |
| 2015 | Research talk at KITP (the Kavli Institute for Theoretical Physics at University of California in Santa Barbara), during the Evoplanets long program. |
| 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 |

- **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.

- **COMMISSIONS OF TRUST**

- 2015 – 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
- 2012 – 2017 Chair of the Graduate Students Award and Jamieson Award committee of the MRP Focus Group
- 2009 – 2011 Member of the AGU Program Committee, on behalf of the MRP Focus Group
- 2009 – 2017 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 – 2017 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, French Fluent
- German, Italian Intermediate