

VALENTINA ERASTOVA

www.erastova.xyz

My research focus is on the use and development of molecular modelling techniques for the study of minerals, materials and interactions at their interfaces. I have a unique multidisciplinary expertise, that allows me to bring together knowledge from theoretical and experimental chemistry, material and geosciences. I aspire for my work to foster a step-change in computational modelling, moving it from its current mostly academic usage to a tool that can directly impact society.

EMPLOYMENT

- 2019
2018
2017
2015
2012
- Chancellor's Fellow**, Erastova group, School of Chemistry, University of Edinburgh, UK
 - PDRA**, group of Dr Paul Hodgkinson, Chemistry Department, Durham University, UK
Combining Molecular Modelling and solid-state NMR for the Study of Organic Crystals, funded by Engineering and Physical Sciences Research Council, UK
 - PDRA**, group of Prof Chris Greenwell, Earth Sciences Department, Durham University, UK
Visiting Researcher, group of Prof Dermot O'Hare, Chemistry Department, University of Oxford and SCG-Oxford Centre of Excellence, UK
 - Molecular Modelling of Low Order Oxide Surfaces for Catalytic Reactions**, personal funding from Siam Cement Group, Thailand
 - PDRA**, group of Prof Chris Greenwell, Earth Sciences Department, Durham University, UK
Visiting Researcher, group of Prof Don Fraser, Earth Sciences Department, University of Oxford, UK
 - Mineral Assisted Formation of Protobiomolecules**, funded by Leverhulme Trust, UK
 - Knowledge Transfer Partnership Research Fellow**, group of Prof Mark Wilson, Chemistry Department, Durham University, UK
 - Mixing and Separation in Polymeric Systems**, in collaboration with P&G, Germany

FUNDING and selected AWARDS

- Chancellor's **Fellowship** Materials and Manufacture, University of Edinburgh (2019–2024)
- SAGES PECRE funding for 2x **visits** to the Universities of Rutgers and Princeton (2019-2020)
- **Founder's Prize** at the British Magnetic Resonance Group Annual General Meeting (2018)
- Siam Cement Group **industrial funding**, Researcher co-Investigator (2015-16, 2016-17)
- **Overseas Research Student Award Scholarship**, personal scholarship covering international PhD tuition fees (2008-13)

PUBLICATIONS and OUTPUT

For publications see erastova.xyz and [Google Scholar](#)

For software see erastova.xyz and [GitHub](#)

For online tutorials and invited Workshops Teaching see erastova.xyz

EDUCATION

- 2013
PhD in Chemistry, Durham University, UK
"Molecular Simulation Studies of Diesel Fuel Crystallisation and Cold Flow Additives"
[thesis under embargo due to industrial interest]
Supervisor: Prof Mark Wilson, Durham University, UK
Funding: Infineum, UK and Overseas Research Student Award
- '08
MChem, Durham University, UK with 1 year on Erasmus Exchange Programme in Spain
Masters Thesis: *"A Computational Study of the Mechanism of the Unimolecular Elimination of unsaturated Aldehydes"*
Supervisor: Prof Jesús Rodríguez-Otero, Universidade de Santiago de Compostela, Spain
Bachelors Thesis: *"Potential Energy Surfaces of Bimolecular Exchange Reactions"*
Supervisor: Dr Eckart Wrede, Durham University, UK
- '07
School of Chemistry and Mathematics No. 574, under supervision of *Russian University of Chemistry and Technology named after D.I. Mendeleev*, Moscow, Russia
- 2002
School of Arts and Design No. 16, Moscow, Russia

POSITIONS of RESPONSIBILITY

- Current
- Member of Editorial Board of [Philosophical Transactions of The Royal Society A](#)
 - Member of Scientific Selection Panel for [HPC-Europa3 Transnational Access Program](#)
 - Member of [UK Centre for Astrobiology](#) and [Centre for Science at Extreme Conditions](#)
 - Reviewer for Journals – see [Publons](#)
 - Scientific Consulting for Filming Industry
 - Thesis committee, *Comité de Suivi Individuel*, IMT Atlantique, France
- Past
- PDRA representative for Faculty of Science and founder of PDRA Committee, reporting to Board of Studies in Chemistry, Durham University, UK
 - Ambassador for *FameLab*, World's leading Science Communication Competition
 - Chair of round table discussions, *Interdisciplinary Origin of Life Meeting*, Germany
 - Chair and Judge at Durham University Chemistry Annual Postgraduate Gala
 - Mentor at University College, Durham University
 - Scientific Editor and later Editor-in-Chief, *Kaleidoscope*, The Interdisciplinary Journal of the *Institute of Advanced Study*, UK
 - Judge at *The Big Bang* Young Scientist and Engineer Fair, North East, UK
 - Member of *Voice of Young Science*, part of *Sense about Science*
 - Freelance scientific translator English-Russian
 - Founding member of *Formulated Product Engineering* Special Interest Group, *IChemE*
- Member
- Associate Fellow of Higher Education Academy, UK
 - Senior Common Room, University College, Durham University, UK
 - Mineralogical Society of Great Britain and Ireland
 - European Association of Geochemistry
 - Royal Society of Chemistry

In MEDIA

- Scientific Comment for Chemistry World News "[Computer says no to membrane-bound life on Titan](#)", by P Hughes (2020)
- Interview on RT "[How did life form from rocks? Protein puzzle reveals secrets of Earth's evolution](#)" (2018)
- Interview at Radio Cardiff program *Pythagoras' Trousers* (2015)
- NOBELini, Live Interview as Selected Scientist (2009)

For more information about our research and current positions see www.erastova.xyz