VALENTINA ERASTOVA

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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

current

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

2017

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

2015

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

2012

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

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

'07

Bachelors Thesis: ***"****Potential Energy Surfaces of Bimolecular Exchange Reactions"*
Supervisor: Dr Eckart Wrede, Durham University, UK

Subjects Studied: Chemistry, Mathematics and Earth Sciences

'04

School of Chemistry and Mathematics 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

FUNDING and AWARDS

- Awarded *Founder's Prize* at the British Magnetic Resonance Group Annual General Meeting (2018)
- Siam Cement Group industrial funding for *Molecular Modelling of Low Order Oxide Surfaces for Catalytic Reactions*, Researcher co-Investigator (2015 – 2016, 2016 – 2017)
- Knowledge Transfer Partnership Research Fellowship in collaboration with P&G (2012)
- Overseas Research Student Award Scholarship, personal scholarship covering international PhD tuition fees (2008 – 2013)

POSITIONS of RESPONSIBILITY

Current

- Thesis committee, Comité de Suivi Individuel, SUBATECH, IMT Atlantique, France
- Chair of round table discussions, Interdisciplinary Origin of Life Meeting, Germany
- Reviewer for Journals: *Minerals, Clay and Clay Minerals, Journal of Physical Chemistry C, Applied Surface Science, Clay Minerals, Minerals Letters*
- Scientific Consulting for Filming Industry
- Mentor and Member of Senior Common Room, University College, Durham University
- Ambassador for *FameLab*, World's leading Science Communication Competition

Past

- 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*

Memberships

- Associate Fellow of Higher Education Academy, UK
- Clay Minerals Society
- European Association of Geochemistry
- Royal Society of Chemistry

TEACHING and SUPERVISION

2018/19

- Invited lectures at International Workshops on the topic of molecular modeling of minerals and materials

2014/19

- Developed and delivered postgraduate course *Practical Simulations for Molecules and Materials*, Chemistry Department, Durham University, UK. Lectures and tutorials are freely available at www.erastova.xyz/teaching

2008/14

- Teaching *Biomolecular modelling, Advanced Computational Chemistry, Computational Physics* and *Chemical Physics* courses for undergraduate students across chemistry degree, Durham University, UK
- Physical Chemistry and Organic Chemistry Laboratory Demonstrator, Durham University, UK
- Tutor in Chemistry for private tutoring company
- Delivery and design of Science Communication Training and a workshop *Physics Tricks and Tricky Physics* at local schools, UK

RESEARCH SUPERVISION:

Will Glossop, PhD (2017-current) *Solid-state NMR and molecular modelling of drug co-crystals*

Shansi Thian, PhD (2016-current) *Evaluation of occurrence, state and mobility of shale oil*

Thomas Underwood, PhD (2013/17) *Molecular dynamics simulations of clay-oil-brine interfaces: understanding low salinity enhanced oil recovery*

Lucas Rudden, MSci (2016/17) *Assessment of force field parameters for mineral interfaces modelling*

James Dix, MChem (2013/14) *Molecular modelling of clay swelling inhibition mechanism*

Laura Krick, BSci (2015/16) *Atomistic modelling of pesticide retention in soils*

Jessica Leung, BSci (2014/15) *Molecular modelling of pesticide – soil interactions*

Kevin Kendaru, BSci (2013/14) *Enhanced oil recovery from the molecular perspective*

Joshua Tasker, BSci (2013/14) *Molecular modelling of low salinity enhanced oil recovery*

Major COLLABORATIONS

Through my work I have established a vast international network of academic and industrial collaborations. I have ongoing projects with *Prof Stewart Clark* (Durham University) on the combined use of MD and planewave DFT for the modeling of material interfaces; *STFC* (UK) on the automation of pipelines in material simulations, *Prof Andrey Kalinichev* (SUBATECH, IMT Atlantique) on the development of parameters for atomistic modeling on minerals. My continuous collaborations with experimental groups of *Prof Franca Castiglione* (Politecnico di Milano), on the study of encapsulated drug molecules through NMR, *Prof Dermot O'Hare* (University of Oxford) and *Prof Karl Coleman* (Durham University) on the creation of high-surface materials, allows for the direct application of my work. Furthermore, my previous and current industrial collaborations with *Infineum* (UK), *BP* (UK), *P*&G (Germany), *Siam Cement Group* (Thailand) and *Applied Graphene Solutions* (UK) allow for further uptake of my research by industries.

In MEDIA

- RT interview *'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)

SELECTED PRESENTATIONS

2018

Invited Lecture at SUBATECH, IMT Atlantique, France *(upcoming)*

Invited Lecture at CeREES, Durham, UK *(upcoming)*

Invited Talk and Chair of Roundtable at Interdisciplinary Origin of Life Meeting, Institut für Molekulare Evolution, Düsseldorf, Germany

Invited Workshop *Molecular Modeling for Polymers and Materials,* Ruhr-Universität Bochum, Germany

Invited Talk at BRSG: Magnetic Resonance Group Annual General Meeting, "Rationalizing dynamics in solids through molecular simulations", Southampton, UK [*Awarded Founder's Prize*]

Departmental Seminar "Computational Chemistry as a Time-Traveller's Tool", Durham, UK

'17

Talk for a broad audience: "Geological origins of Life on Earth and Beyond", Goldschmidt, Paris, France

Oral presentation, International Clay Conference, Granada, Spain

Invited Workshop Lectures on Computational Modeling of Clay Mineralogy, ASYS-AIPEA School for Young Scientist, Granada, Spain

'16

Invited Talk, CECAM *Atomistic simulations in prebiotic chemistry – a dialog between experiment and theory*, University Pierre and Marie Curie, Paris, France

'15

Invited Talk, Layered Double Hydroxide Symposium, University of Oxford, UK

Oral presentation, CECAM *Atomistic simulations in Earth Sciences*, University Pierre and Marie Curie, Paris, France

'14

Oral presentation, EuroClay, Edinburgh, UK

Invited Oral Presentation, Computational Chemistry Sessions, Magdalen College, University of Oxford, UK

Invited Lecture, St Petersburg State University, Russia

'13

Invited Talk, CECAM school *Multiscale simulations of Soft Matter with VOTCA*, Max Planck Institute for Polymer Research, Mainz, Germany

'10

Oral presentation, CECAM *Corse graining multicomponent soft matter*, Johannes Gutenberg University, Mainz, Germany

2009

The Scientist Selection at NOBELini, Medical Research Council and Central Saint Martins, UK

PUBLICATIONS

* First Author; ✉ Corresponding Author; ⇒ Key Publications, discussed.

⇒ **V Erastova***✉, K Ruengkajorn*, JC Buffet, HC Greenwell & D O'Hare, "Aqueous Immiscible Layered Double Hydroxides: Synthesis, Characterisation and Molecular Dynamics Simulation", *ChemComm,* 2018

> Layered double hydroxides have gained popularity for use as catalysts and supports, adsorbents, polymer additives and flame retardants. While their synthesis is straightforward, it often yields materials with undesirable low-surface areas. A post-synthesis treatment with aqueous miscible solvents for delamination and dispersion of hydroxide layers, leading to up to 40x larger surfaces, has been previously reported. In this work, we use molecular dynamics to rationalise the mechanism behind delamination process and demonstrate that atomic information gathered by simulation can be exploited to successfully identify solvents having desirable effects at the macroscopic scale. Front cover by V Erastova, Referee Recommended Article, HOT ComChem list.

- S Tian, **V Erastova**, S Lu, HC Greenwell, T Underwood, H Xue, F Zeng, G Chen & C Wu, "Understanding model crude oil component interactions at kaolinite silicate and aluminol surfaces: towards improved shale oil recovery", *Energy and Fuels,* 2017

⇒ **V Erastova**✉, MT Degiacomi, DG Fraser & HC Greenwell, "Mineral Surface Chemistry Control for Origin of Prebiotic Peptides", *Nature Communications,* 2017

> In this article, we examine the role layered hydroxides (LDH) could have played in prebiotic peptide formation. We modelled processes under early Earth conditions, difficult to attain experimentally. We demonstrate how LDHs can concentrate, align and act as adsorption templates for amino acids and, during wetting-drying cycles, promote peptide bond formation. We propose a testable mechanism for the spontaneous growth of peptides in early Earth. Overall, our results are the first to demonstrate the potential role of mineral surfaces in mimicking aspects of biochemical reaction pathways. This work has been features in media.

- **V Erastova**✉, MT Degiacomi, D O'Hare & HC Greenwell, "Understanding Surface Interactions in Aqueous Miscible Organic Solvent Treated Layered Double Hydroxides", *RSC Advances,* 2017
- T Underwood, **V Erastova** & HC Greenwell, "Clay adsorption at smectite clay mineral surface", *Clays and Clay Minerals,* 2016
- **V Erastova***✉, MT Degiacomi* & MR Wilson, "Easy creation of polymeric systems for molecular dynamics with *Assemble!*", *Computer Physics Communications,* 2016
- **V Erastova***, B Grégoire*, DL Geatches, SJ Clark, HC Greenwell & DG Fraser, "Insights into the Behaviour of Biomolecules on the Early Earth: The Concentration of Aspartate by Layered Double Hydroxide Minerals", *Geochimica et Cosmochimica Acta,* 2016
- T Underwood, **V Erastova** & HC Greenwell, "Wetting Effects and Molecular Adsorption at Hydrated Kaolinite Clay Mineral Surfaces", *The Journal of Physical Chemistry C,* 2016

⇒ T Underwood, **V Erastova**, P Cubillas & HC Greenwell, "Molecular Dynamic Simulations of Montmorillonite-Organic Interactions under Varying Salinity: An Insight into Enhanced Oil Recovery", *The Journal of Physical Chemistry C,* 2015

> Enhanced Oil Recovery (EOR) is a technique used to maximise oil fields production. One of the most widely used EOR methods relies on injecting partially desalinated marine water into the well. Although routinely used, the fundamental underlying chemistry of this process is still not understood. In this seminal paper, we use large scale molecular simulations to study interactions between oil components, various oil fractions with common clays in various environments. This work has triggered further investigations by the computational geoscience research community, and has been cited 30 times in the first 2 years.

- **V Erastova**, J Rodríguez-Otero, EM Cabaleiro-Lago & A Peña-Gallego, "A computational study of the mechanism of the unimolecular elimination of *α,β*-unsaturated aldehydes in the gas phase", *Journal of Molecular Modeling,* 2011