Valentina Erastova

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EMPLOYMENT

Aug 2025 -: **Senior Lecturer**, School of Chemistry, University of Edinburgh, UK.

2023 – 25: **Lecturer**, School of Chemistry, University of Edinburgh, UK.

2019 – 25: **Chancellor's Fellow** in Materials & Manufacture, School of Chemistry, University of Edinburgh, UK.

2018 – 19: **PDRA**, *Combining Molecular Modelling and Solid-State NMR for the Study of Organic Crystals,* group of Prof. Paul Hodgkinson, Chemistry Department, Durham University, UK.

2015 – 17: **PDRA**, *Molecular Modelling of Low Order Oxide Surfaces for Catalytic Reactions,* group of Prof. Chris Greenwell, Earth Sciences Department, Durham University, UK, and Visiting Researcher group of Prof. Dermot O'Hare, Chemistry Department, University of Oxford, UK, and SCG-Oxford Centre of Excellence; funded by *Siam Cement Group*, Thailand (Researcher co-applicant).

2013 – 15: **PDRA**, *Mineral Assisted Formation of Protobiomolecules,* group of Prof. Chris Greenwell, Earth Sciences Department, Durham University, UK.

2012: **Knowledge Transfer Partnership Research Fellow**, *Mixing and Separation in Polymeric Systems,* group of Prof. Mark Wilson, Chemistry Department, Durham University, UK; funded by *P&G*, Germany.

EDUCATION

2008 – 13: **PhD** in Chemistry, Durham University, UK. Title: *Molecular Simulation Studies of Diesel Fuel Crystallisation and Cold Flow Additives*, supervised by Prof. Mark Wilson; funded by *Infineum*.

2004 – 08: **MChem**, Durham University, UK, with Erasmus Exchange at the Universidade de Santiago de Compostela, Spain, Title: *A Computational Study of the Mechanism of the Unimolecular Elimination of α,β-unsaturated Aldehydes*, supervised by Prof. Jesus Rodriguez-Otero.

AWARDS

2021: **Principal's Medal for Exceptional Contribution** for the *Scientist Next Door* initiative.

2018: **Founder's Prize** by the British Magnetic Resonance Group.

2008 – 13: **Overseas Research Student Award Scholarship**.

FUNDING

Fellowships/Grants:

2019 – 25: Chancellor's Fellowship Materials and Manufacture. 5-year Independent Fellowship from the Scottish Funding Council, awarded by the University of Edinburgh.

2015 – 17: Siam Cement Group industrial funding for *Molecular Modelling of Low Order Oxide Surfaces for Catalytic Reactions*. Research co-applicant, Postdoctoral Funding, 2 years.

Computational Resources:

Computing time on the Tier 1 and Tier 2 computing facilities, secured application to UKRI.

2024 – 25: *Quantifying Soil-Organic Interactions on Rocky Planets*. Access to Isambard3, awarded by UKRI.

2024 – 25: *Developing molecular models of biochar porosity*. Access to Cirrus, awarded by EPSRC.

2023 – 24: *Molecular simulations of nano-confined fluids in clay mineral and organic matter pores*. Access to BEDE (co-I, PI Chris Greenwell, Durham University)

2023 – 24: *Understanding interactions between drug pollutants and charcoals through molecular modelling*. Access to Cirrus HPC, awarded by EPSRC.

2022 – 23: *Emergence of sequence in a prebiotic mineral-assisted peptide growth*. Access to BEDE HPC (co-I, PI Matteo Degiacomi, Durham University)

2021 – 22: *Understanding interactions between drug pollutants and soil*. Access to Cirrus.

PhD studentships:

2023: *Understanding interactions between minerals and small biopolymers under extreme conditions*. School of Chemistry and School of Physics and Astronomy joint funding to support the Centre for Science at Extreme Conditions.
2023: *Understanding Preservation of Potential Biosignatures by Martian Soils*. E4 DTP.
2020: *Molecular Modelling to Aid Design of Biochar Materials*. E4 DTP.

Other Fundings:

2025: *EnviroForum.* Support from the Futures Institute to develop an AI app used for UG taught degrees.
2023: *Molecular modelling of soils for nuclear waste management.* Scottish Funding Council Saltire Emergent Researcher Scheme.
2022: *Iterative Approach for Creation of Biochar Molecular Models.* Equipment grant, by ScotChem.
2022: *Effect of cometary dust on ice growth.* HPC Europa transnational exchange. (co-I, PI Carmen Biaino)
2021: RSC Outreach Award to support the Scientist Next Door project.
2021: *Modelling the reactivity at interstellar ice and mineral interfaces for prebiotic molecules formation and condensation: unveiling the mysterious appearance of life bricks on Earth.* HPC Europa transnational exchange. (co-I, PI Carmen Biaino, SNS Pisa)
2020: RSC Outreach Award to support the Scientist Next Door project.
2019: *Multi-scale Modelling of ancient Earth.* HPC Europa transnational exchange. (co-I, PI Kenneth McGuinness, Rutgers University)
2019: PECRE travel grant to support collaboration with Prof Yee, Rutgers University, USA. Scottish Funding Council.

SUPERVISION

As first supervisor:

2023 – : Sarah Stewart, PhD student.
2021 – 25: Audrey Noumbissi-Ngambia, PhD student.
2021 – 25: Hannah Pollak, PhD student. Submitted.
2020 – 24: Rosie Wood, MScR with distinction. (Rosie is now a research scientist at Alan Turing Institute.)

As co-supervisor:

2022 – : Jacub Licko, PhD student, 1st supervisor Prof. Kalinichev, IMT Atlantique, France.
2023 – 24: Omar Nuruzade, Masters, 1st supervisor Prof. Dong, University of Maimi, USA.
2021 – 24: Rixin Zhao, PhD student, 1st supervisor Prof. Lu, School of Geosciences in China University of Petroleum, China. (Rixin is now a tenure-track at Yangtze University, China.)

UG Project supervision:

2019 – : 10 BSci, 2 MChem at Edinburgh, 8 MChem abroad/industry.

PG Taught Masters supervision:

2019 – : 9 projects, 4 literature reviews.

TEACHING

Full details on my teaching activities are outlined in the **Teaching Statement**.

At the University of Edinburgh:

2023 – : ***Research Techniques Computational Chemistry*** 40% of a module, SCQF 11, PgT, 20 credits, 3 cohorts of 20+ students per year. (Corse materials via GitHub, publication in review - article proof)
2021 – : ***Data-Driven Chemistry*** module, SCQF level 8, 2nd year UG, 20 credits, mandatory, 120+ students per year. (Corse materials via GitHub, Associated publication DOI: 10.21105/jose.00192)
2020 – : ***Origins of Elements*** lectures, tutorials and workshops part of the *Environmental Chemistry* module, SCQF level 8, 2nd year UG, elective, 60-100 students per year.
2020 – 21: ***Python for Chemists*** module to replace chemistry laboratories for all 2nd and 3rd year UG students during COVID.
2023 – : **Laboratories** in *Physical Chemistry* 3rd year, *Inorganic Chemistry* 2nd year, and *Environmental Chemistry* 2nd year.
2019 – 23: **Tutorials** for the 2nd year Inorganic Chemistry.

External Teaching:

Jan 2025: Invited lecture for the ***Virtual Winter School on Computational Chemistry*** (https://winterschool.cc), entitled *Computational Chemistry – Space & Time Travellers Tool*, recordings DOI: 10.5281/zenodo.14938180. (Most downloaded/viewed talk of the School)

2024 – : Lecturer for ***Biochar Virtual Lecture Series,*** hosted by the *International Biochar Initiative* (https://biochar-international.org), starting bi-weekly from February 2025.

2023 – : ***Computational Methodologies for Astrobiology Research*** for Scottish Universities Physics Alliance *Astrobiology* course.

ACADEMIC LEADERSHIP

2025 – : **Cohort Lead for Physical Chemistry** (Supporting UG students in Years 1-5 during their degree).

2024 – 25: **Chair** of the School of Chemistry *Student Allocation Committee*. (Managing allocation of EPSRC DLA and other PhD funds within the School.)

2023 – : **Lead** for the *Climate and Sustainability* research theme of the School of Chemistry.

2023 – : **Lead** for the *Energy, Environmental and Sustainable Chemistry* research theme at EaStCHEM (joint Schools of Chemistry at the Universities of Edinburgh and St. Andrews).

2023 – 24: **Member** of the School of Chemistry *Research Committee*.

2021 – 24: **Member** of the School of Chemistry *Student Allocation Committee*. (Contribution to the decision on the EPSRC DTP/DLA PhD student allocations within the School.)

2022 – : **Member** of the *University's Research Computing and Analytical Environments Advisory Group*. (Recommendations on computing facility management and upgrades for the University.)

2019 – : **Representative** for the School of Chemistry at the NERC E4/E5 DTP steering committee and the SOFI2 CDT steering committee.

2019 – : **Member of the Editorial Board** of the *Philosophical Transactions of the Royal Society A*, Royal Society Publishing.

2018 – : **Founding member** of the OoLEN – *Origin of Life Early Career Network*. (Coordination of international meetings, and community publications in peer-reviewed journals.)

2019 – 22: **Chair** of *Scientific Selection Panel* for *HPC Europa Transnational Access* (international programme to facilitate visits between the main HPC centres in Europe, funded by Horizon 2020).

COMMISSION OF TRUST

PhD examiner:

- Nil Gaudu, Nitschke-Duval Group, CNRS Marseille, France (upcoming 2025).
- Carmen Biaino, Barone group, Scuola Normale Superiore Pisa, Italy (2023).
- Kyle Acheson, Kirrander group, School of Chemistry, University of Edinburgh (2023).
- Michail Papadourakis, Michel group, School of Chemistry, University of Edinburgh (2021).
- Liam Perera, Cockell group, School of Physics and Astronomy, University of Edinburgh (2021).
- Ellie Tanaka, Robertson group, School of Chemistry, University of Edinburgh (2020).
- Annual reviews, PhD thesis committee, Comité de Suivi Individuel, IMT Atlantique, France (since 2019).

Reviewer for:

- Scientific Journals, incl. JACS, Chemical Engineering Journal, Chemical Geology, ACS Earth and Space Chemistry, PLOS One, Applied Surface Science, Clays and Clay Minerals, Journal of Physical Chemistry, Molecular Liquids, Langmuir, Clay Minerals, Energy & Fuels, Computer Physics Communications, Astrobiology, International Journal of Astrobiology, Cell Reports.
- Elsevier Book Publishing: Submissions on topics of Astrobiology/Space and Planetary Science.
- Funding Bodies: EPSRC, Polish Academy of Science, NASA NSPIRES Space Technology Mission Directorate.
- Member of the NERC *College of Science and Engineering* Review Panel.

Memberships:

- Member of the Royal Society of Chemistry (since 2019).
- Origin of Life Early Career Network (since 2018, founding member).
- Scottish Alliance for Geosciences, Environment and Society (since 2019).
- Associate Fellow Higher Education Academy (since 2015).
- European Association of Geochemistry (since 2015).
- AIPEA - Association Internationale pour l'Étude des Argiles (since 2015).
- Mineralogical Society of the UK and Ireland (since 20215)
- CCP5 (since 2010).

Visiting Academics:

- Mehdi Ghasemi, University of Manchester, 2-moonth project funded by Clay Minerals Society. (2025)
- Omar Nuruzade, 6-month visiting student from Khazar U., Azerbaijan. (2022 – 23)
- Carmen Biaino, 6-month visiting PhD from Dr Tasinato group, SNS Pisa. (2021 – 22)
- Dr Kenneth McGuinnes, 3-month visiting PDRA from Prof Yee group, Rutgers U. (2022)

ORGANISATION OF EVENTS

July 2025: **Lead convenor** of *The Role of Layered Minerals in the Origin of Life – Insights from Terrestrial and Extraterrestrial Environments* session at the International Clay Conference, Dublin, Ireland.

June 2025: **Lead organiser** of CECAM workshop *Advancing biochar molecular models – from experiments to model construction and application*, Lausanne, Switzerland.

Jan. 2025: **Co-organiser** of the *Recent Appointees in Physical Chemistry* meeting of RSC Faraday Council hosted at the University of Edinburgh, UK.

May 2024: **Lead organiser** of the *Molecular Modelling in Clay Science* (https://molecular-clay-meeting.uk), a 2-day international meeting and a workshop of the Mineralogical Society of UK and Ireland, hosted at the University of Edinburgh, UK.

2020: **Co-organiser** of the *Building Worlds* seminar series of the UK Centre for Astrobiology.

INVITED PRESENTATIONS

Since starting my independent position at the University of Edinburgh in 2019, I have been invited to deliver *7 departmental seminars in the UK* (St Andrews, Birmingham, Durham, Royal Holloway, Harriot-Watt and Bristol Universities), *9 seminars internationally* (Université Paris-Saclay, Chimie ParisTech – PSL, Khazar University, Ruđer Bošković Institute, IMT Atlantique, Rugers University and Princeton University), *14 talks at international conferences/meetings* (incl., Goldschmidt, 6th Manchester Multiscale conference, GeoMinKöln, CANUK, Forming and Exploring Habitable Worlds), *2 lectures at international schools* (CCP5 and Virtual Winter School on Computational Chemistry), *5 presentations at industrial events*, and *2 academic training workshops*.

OUTREACH

Throughout my scientific career, I have been actively engaging in numerous activities to disseminate science to broader audiences, below are some examples of my recent activities:

- Invited presentations about my research at various events, such as *Pint of Science* (Edinburgh, 2023) or as a public seminar jointly hosted by Khazar and French-Azerbaijani Universities (Baku, Azerbaijan, 2024), attended by students and a broad public audience.
- Interviews on the radio (Radio Cardiff program *Pythagoras' Trousers,* 2015) and in the press (RT interview *'How did life form from rocks?' Protein puzzle reveals secrets of Earth's evolution*, 2018).
- Invited article for the general scientific audience "*Unveiling secrets of the microscopic world: molecular modelling in clay science*" for *Philosophical News* (2024, Issue 1) of the Clay Minerals Group.
- Invited comments on recent scientific publications for general articles published in Chemistry World, New Scientist, C&EN, MIT Technology Review, Live Science (e.g.: *Glass flask catalysed famous Miller-Urey origin-of-life experiment* (2021), *Algorithm discovers how six simple molecules could evolve into life's building blocks* (2020), *Computer says no to membrane-bound life on Titan* (2020), *What could aliens look like?* (2024)).
- Founder of the Scientist Next Door project in response to the COVID-19 pandemic, which connected 100+ scientists from across the globe with their local pupils. To support the management and operation of this project, I have secured funding from the Institute of Biophysics (£3K) and RSC Outreach funding (2x £5K). The Scientist Next Door has been covered in media (incl. Northern Echo, Palatinate, Viral Stories). For the impact made through this initiative to the local population, I was awarded the ***Principal's Medal for Exceptional Contribution*** in 2021.

PUBLICATIONS (selected)

Below, I present only publications since moving into my independent position at the University of Edinburgh in July 2019. The full list of my publications can be found on Google Scholar. ***** indicates publications where I appear as (co-)corresponding author, and blue highlights members of my research group.

1. Zhentao Dong, Shansi Tian, Haitao Xue, Shuangfang Lu, Bo Liu, Valentina Erastova, Guohui Chen, Yuying Zhang. "A novel method for automatic quantification of different pore types in shale based on SEM-EDS calibration." Marine and Petroleum Geology, 173, (**2025**): 107278. DOI: 10.1016/j.marpetgeo.2024.107278.
2. Hannah Pollak, Matteo T. Degiacomi, and Valentina Erastova*. "Modelling realistic clay systems with ClayCode." *Journal of Chemical Theory and Computation* 20, no. 21 (**2024**): 9606–9617. DOI: 10.1021/acs.jctc.4c00987. **Cover article**.
3. Zhentao Dong, Shansi Tian, Haitao Xue, Shuangfang Lu, Bo Liu, Valentina Erastova, Min Wu, Rongyue Fu, "Analysis of Pore Types in Lower Cretaceous Qingshankou Shale influenced by Electric Heating." *Energy & Fuels,* 38, no. 21 (**2025**): 20577–20590. DOI: 10.1021/acs.energyfuels.4c03783.
4. Rixin Zhao, Haitao Xue, Shuangfang Lu, H. Chris Greenwell, and Valentina Erastova*. "Molecular dynamics of quantitative evaluation of confined fluid occurrence characteristics in nanopores media and the influencing mechanism: pore size and pore geometry." *Physics of Fluids* 36, no. 9 (**2024**): 092027. DOI: 10.1063/5.0226864.
5. Sarah V. Stewart and Valentina Erastova*. "Understanding the Role of Layered Minerals in the Emergence and Preservation of Proto-Proteins and Detection of Traces of Early Life." *Accounts of Chemical Research* 57, no. 17 (**2024**): 2453–2463. DOI: 10.1021/acs.accounts.4c00173. **Cover article**; featured in SoC news; featured in Astrobiology Web **news**.
6. Valentina Erastova, Ivana R. Evans, William N. Glossop, Songül Guryel, Paul Hodgkinson, Hannah E. Kerr, Vasily S. Oganesyan, Lorna K. Softley, Helen M. Wickins, and Mark R. Wilson. "Unravelling guest dynamics in crystalline molecular organics using 2H solid-state NMR and molecular dynamics simulation." *Journal of the American Chemical Societ,* 146, no. 27 (**2024**): 18360–18369. DOI: 10.1021/jacs.4c03246.
7. Rixin Zhao, Haitao Xue, Shuangfang Lu, H. Chris Greenwell, and Valentina Erastova*. "Revealing crucial effects of reservoir environment and hydrocarbon fractions on fluid behaviour in kaolinite pores." *Chemical Engineering Journal*, 489 (**2024**): 151362. DOI: 10.1016/j.cej.2024.151362
8. Audrey Ngambia, Ondřej Mašek, and Valentina Erastova*. "Development of biochar molecular models with controlled porosity." *Biomass and Bioenergy* 184 (**2024**): 107199. DOI: 10.1016/j.biombioe.2024.107199.
9. Rosie Wood, Ondřej Mašek, and Valentina Erastova*. "Developing a molecular-level understanding of biochar materials using public characterization data." *Cell Reports Physical Science* 5, no. 7 (**2024**): 102036. DOI: 10.1016/j.xcrp.2024.102036.
10. Rosie Wood, Ondřej Mašek, and Valentina Erastova*. "Developing realistic molecular models of biochars." *Cell Reports Physical Science* 5, no. 7 (**2024**): 102037. DOI: 10.1016/j.xcrp.2024.102037.
11. Omar Nuruzade, Elshan Abdullayev, and Valentina Erastova*. "Organic–Mineral Interactions under Natural Conditions: A Computational Study of Flavone Adsorption on Smectite Clay." *The Journal of Physical Chemistry C* 127, no. 27 (**2023**): 13167–13177. DOI: 10.1021/acs.jpcc.3c00174.
12. James Cumby, Matteo T. Degiacomi, Valentina Erastova, J. Jasmin Güven, Claire L. Hobday, Antonia S. J. S. Mey, Hannah Pollak, and Rafal Szabla. "Course materials for an introduction to data-driven chemistry." *Journal of Open Source Education* 6, no. 63 (**2023**): 192. DOI: 10.21105/jose.00192.
13. Stuart J. Goldie, Matteo T. Degiacomi, Shan Jiang, Stewart J. Clark, Valentina Erastova*, and Karl S. Coleman. "Identification of Graphene Dispersion Agents through Molecular Fingerprints." *ACS Nano* 16, no. 10 (**2022**): 16109-16117. DOI: 10.1021/acsnano.2c04406.
14. Shansi Tian, Zhentao Dong, Bo Liu, Haitao Xue, Valentina Erastova, Min Wang, and Haiyang Yan. "Characteristics of gaseous/liquid hydrocarbon adsorption based on numerical simulation and experimental testing." *Molecules* 27, no. 14 (**2022**): 4590. DOI: 10.3390/molecules27144590.
15. Matteo T. Degiacomi, Shansi Tian, H. Chris Greenwell, and Valentina Erastova*. "*DynDen*: Assessing convergence of molecular dynamics simulations of interfaces." *Computer Physics Communications* 269 (**2021**): 108126. DOI: 10.1016/j.cpc.2021.108126.
16. Shansi Tian, Leon Bowen, Bo Liu, Fang Zeng, Haitao Xue, Valentina Erastova, H. Chris Greenwell, Zhentao Dong, Rixin Zhao, and Jinzhong Liu. "A method for automatic shale porosity quantification using an Edge-Threshold Automatic Processing (ETAP) technique." *Fuel* 304 (**2021**): 121319. DOI: 10.1016/j.fuel.2021.121319.
17. Martina Preiner, Silke Asche, Sidney Becker, Holly C. Betts, Adrien Boniface, Eloi Camprubi, Kuhan Chandru, Valentina Erastova, Sriram G. Garg, Nozair Khawaja, Gladys Kostyrka, Rainer Machné, Giacomo Moggioli, Kamila B. Muchowska, Sinje Neukirchen, Benedikt Peter, Edith Pichlhöfer, Ádám Radványi, Daniele Rossetto, Annalena Salditt, Nicolas M. Schmelling, Filipa L. Sousa, Fernando D. K. Tria, Dániel Vörös and Joana C. Xavier. "The future of origin of life research: bridging decades-old divisions." *Life* 10, no. 3 (**2020**): 20. DOI: 10.3390/life10030020.

18. Preprint: OoLEN, Silke Asche, Carla Bautista, David Boulesteix, Alexandre Champagne-Ruel, Cole Mathis, Omer Markovitch, Zhen Peng, Alyssa Adams, Avinash Vicholous Dass, Arnaud Buch, Eloi Camprubi, Enrico Sandro Colizzi, Stephanie Colón-Santos, Hannah Dromiack, Valentina Erastova, Amanda Garcia, Ghjuvan Grimaud, Aaron Halpern, Stuart A Harrison, Seán F. Jordan, Tony Z Jia, Amit Kahana, Artemy Kolchinsky, Odin Moron-Garcia, Ryo Mizuuchi, Jingbo Nan, Yuliia Orlova, Ben K. D. Pearce, Klaus Paschek, Martina Preiner, Silvana Pinna, Eduardo Rodríguez-Román, Loraine Schwander, Siddhant Sharma, Harrison B. Smith, Andrey Vieira, Joana C. Xavier, "What it takes to solve the Origin(s) of Life: an integrated review of techniques." ArXiv (**2023**). DOI: arXiv:2308.11665.
19. Preprint: Sarah V Stewart, Hannah Pollak, Tim J Spankie, Audrey Ngambia, Angela Chitzanidi, Valentina Erastova*. “Course Materials for an Introduction to Computational Chemistry Techniques.” (**2025**). Article proofs on JOSE, under review.

SOFTWARE & RESOURCES

Software:

- ***ClayCode*** (2024)
  github.com/Erastova-group/ClayCode
  DOI: 10.1021/acs.jctc.4c00987.
- ***DynDen*** (2021)
  github.com/Erastova-group/DynDen
  DOI: 10.1016/j.cpc.2021.108126.
- ***Assemble!*** (2015)
  github.com/Erastova-group/Assemble
  DOI: 10.1016/j.cpc.2015.12.026.

Datasets and Models:

- **Porous Biochar Molecular Models** (2024)
  github.com/Erastova-group/Porous_Biochars_Models,
  DOI: 10.1016/j.biombioe.2024.107199.
- **Biochar Molecular Models** (2023)
  github.com/Erastova-group/Biochar_MolecularModels,
  DOI: 10.1016/j.xcrp.2024.102037.
- **Biochar Datasets** (2023)
  github.com/Erastova-group/Biochar_MolecularModels,
  DOI: 10.1016/j.xcrp.2024.102036.

Educational Materials:

- **Data-Driven Chemistry** (2022)
  github.com/Edinburgh-Chemistry-Teaching/Data-driven-chemistry,
  DOI: 10.21105/jose.00192.
- **Research Techniques Computational Chemistry** (2024)
  github.com/Edinburgh-Chemistry-Teaching/MD_ResearchTechniques.
  Preprint: on JOSE.
- ***ClayCode* Workshop Material** (2024)
  github.com/Erastova-group/ClayCode-workshop.