Dr Charlie Wand

E-mail: c.wand[at]exeter.ac.uk

Website: www.charliewand.com

Research Profile

***December 2021 – present* – Lecturer (Education & Research) in Natural Sciences, University of Exeter, UK**

***January 2018 – December 2021* – Postdoctoral Research Associate, Department of Chemical Engineering and Analytical Science (CEAS), The University of Manchester, UK**

- Working with Professors Paola Carbone and Flor Siperstein, I use multiscale modelling to investigate how the nano- and meso- scale structures of soft materials affect bulk properties.
- Part of two EPSRC funded Prosperity Partnerships with industrial collaborators; The Centre in Advanced Fluid Engineering for Digital Manufacturing (CAFE4DM) between The University of Manchester, Unilever, University of Cambridge, STFC (£3.0M), and Sustainable Coatings by Rational Design (SusCoRD) between The University of Manchester, AkzoNobel/International Paint, University of Sheffield (£2.5M).

***April 2016 – December 2017* – Postdoctoral Research Associate, Department of Chemistry, University of Cambridge, UK**

- Part of the BP International Centre for Advanced Materials (BP ICAM), a joint centre between BP, Imperial College, The University of Manchester, the University of Cambridge, and the University of Illinois at Urbana-Champaign (£82M).
- I investigated the of the solubility of asphaltenes (large polyaromatic compounds found in crude oil) using free energy calculations via Monte Carlo, Molecular dynamics and hybrid MC-MD simulations within Professor Daan Frenkel's group.

***January 2015 - January 2016* – Postdoctoral Researcher, Swedish School of Textiles, University of Borås (Sweden)**

- Part of a collaboration between the University of Borås and the University of Skövde funded by Region Västra Götaland, "Design, textiles and sustainable development".
- Within Professor Kim Bolton's group I developed a new computational approach to investigate the molecular-level mechanism for thermal actuation observed in semi-crystalline poly(vinylidene fluoride) and polyethylene using molecular dynamics.
- As part of a collaboration with TetraPak and AB Borealis, I used molecular dynamics and Gibbs Ensemble Monte Carlo to investigate permeation in polyethylene-clay nanocomposites.

***October 2009 – September 2013*– PhD, Department of Chemistry, University of York (UK)**

- EPSRC-DTA funded PhD titled "Monte Carlo simulations of confined nematic systems", supervised by Dr Martin Bates.

***2005 - 2009* – MChem, St. Hilda's College, University of Oxford (UK)**

- Master of Chemistry (Upper Second).

Visiting positions

***September 2019* - Visiting researcher at Sofia University, Bulgaria (10 day stay)**

- Collaboration with Professor Peter Kralchevsky and Professor Krassimir Danov, Department of Chemical and Pharmaceutical Engineering, Sofia University about surfactant theory.

***August 2016* - Visiting research fellow at the University of Borås, Sweden (5 day stay)**

- Collaboration with Professor Kim Bolton and Dr Abas Mohsenzadeh, Department of Engineering about semi-crystalline polymer actuators.

Grant Awards

2021 – ARCHER2 Tier-1 High Performance Computing (HPC) resources (£2,400)

- Scientific Lead and lead grant writer

2018-2019 - Cirrus (EPCC) Tier-2 High Performance Computing (HPC) resources (£15,202)

- Scientific Lead and lead grant writer

2018 - Royal Society of Chemistry Travel Grant for LGBTSteminar, University of York (£100)

2017 **-** BP ICAM additional continuation funding (ca. £86,000)

- 8 month continuation of position at the University of Cambridge awarded following a grant proposal.

Awards

2022 – American Chemical Society C&EN Trailblazer LGBTQ+ Chemist

- One of 18 profiles, of which only 2 were from the UK.

2021 – Winner of the Lionel Shrier prize for best oral presentation by a Young Scientist at the Corrosion Science Symposium and Advances in Corrosion Protection by Organic Coatings from the UK Institute of Corrosion.

2020 – Shortlisted for FSE Better World Award Emerging Impact, The University of Manchester

2019 – Winner CEAS Social Responsibility Award (2018/2019) for Public Engagement/Widening Participation

- Awarded for increasing the visibility and participation of the LGBT+ (Lesbian, Gay, Bisexual and Trans) community in STEM (Science, technology, engineering and maths) subjects

2019 – Winner of CAFE4DM 'Dragon's Den' Competition, The University of Manchester

- Competition for PDRAs to pitch a proposal for a small project (up to 1 year PDRA time) to Unilever and academic representatives
- Awarded for the proposal "Investigating the refreezing of ice cream using computer simulation"

2009 – Winner of the ExxonMobil Prize for Physical and Theoretical Laboratory Undergraduate work, University of Oxford

- Awarded for overall performance over three years in physical and theoretical undergraduate laboratory course to top ~5 students.

Professional Membership

2022 – present Member of the American Chemical Society

2021 – present The Royal Society of Chemistry Statistical Mechanics and Thermodynamics (SMTG) committee member

2020 – present Associate member of The European Materials Modelling Council

2019 - present Member of The Royal Society of Chemistry (Associate Member since 2006)

2018- present Member of CCP5

Technical Proficiencies

Simulation techniques

- Molecular dynamics, Monte Carlo, dissipative particle dynamics, free energy calculations

Coding and scripting Languages

- Fortran – Fluent
- Bash – Proficient
- Python – Proficient, training by University of Cambridge (2017) and MOOC (2014)
- RMake – Beginner, training by The University of Manchester (2019)

Experience with pre-existing software

- Open source simulations: LAMMPS (including additional plugins such as Plumed, PyRETIS), MCCCS Towhee, VMD, Packmol, Gromacs
- Commercial packages: Biovia Materials Studio, NSCCS Scienomics

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Continuing Professional Development (CPD) – Selected

2021– Invisible Dyslexia Training Course, The British Dyslexia Association
2021– Managing at Manchester for Researchers, The University of Manchester certified by the Institute of Leadership & Management (ILM)
2020 – 2021 Leadership in Education Awards Programme (LEAP), The University of Manchester

Teaching Experience

December 2021-present **– Lecturer (Education & Research) in Natural Sciences, University of Exeter**

- Module co-leader for NSC1004: Experimental Science, and NSC3003: Group Project.
- Lecturer on NSCM007: Advanced Topics in Natural Sciences Chemistry II.
- Guest lecturer on LGBT+ inclusion in Science, part of 'Science Skills and Culture' for Foundation programme within the College of Engineering, Mathematics and Physical Sciences.

September 2021**– Fellow of Advance HE (FHEA)**
October 2019-January 2020 **– Teaching Internship Lecturer, The University of Manchester**
Supervision/co-supervision of:

- 3 PhD students in Chemical Engineering and Physics (The University of Manchester, University of Exeter).
- 1 visiting PhD student in Chemistry (University of Cambridge).
- 3 MEng research projects in Chemical Engineering (The University of Manchester).
- 2 MSc projects in Natural Sciences (University of Exeter).
- 2 BSc projects in Chemistry and Natural Sciences (University of York, University of Exeter).
- 3 undergraduate summer internships (University of Exeter).

Outreach and community engagement activities (selected)

Invited talks

February 2022 – "Transitions in Science" LGBTQ+ History Month, PRISM Exeter
June 2021 – Being #CompChemURG: How Diversity Enriches Us, The Binding Site, A community for underrepresented groups in computational chemistry, Global launch attended by ca. 240 participants
February 2020 – Being Queer in Academia: Defying Expectations, University of Nottingham
November 2019 – Gender Diversity Day, Department of Physics & Astronomy, The University of Manchester
November 2019 – Queer in Academia, University of St Andrews
September 2019 – Diversity Challenge, Royal Institution, London

Media Appearances

June 2022 – Featured in "The Queer Variable" a free e-book by Dr Alfredo Carpineti and Dr Shaun O'Boyle, funded by Science Foundation Ireland and The Physiological Society for Pride in STEM.
https://prideinstem.org/the-queer-variable/
January 2022 – LGBTQ+ ChemEs & Allies profile for the American Institute of Chemical Engineers (AIChE)
June 2021 – Profile for Schools OUT UK, a UK-based charity focussing on LGBT inclusion in schools.
February 2020 – Podcast for https://www.realscientistsnano.org/ on materials/nano science

Online activities

June 2021 – Featuring in @QueerEngineers Twitter campaign about LGBT+ Engineers
November 2020 – Taking part in the Global Science show on Twitter talking about surfactants
February 2020 – Curating @RealSci_Nano Twitter account for one week, promoting materials/nano science.

Other

2022-present – Grants panel member for the LGBT+ Future: Bi Fund from the LGBT Consortium
2022-present – Volunteer organiser for PRISM Exeter, a local network for LGBTQ+ in STEMM
2022 – Science outreach to a LGBTQ+ youth group including development of hands-on activities.