James P. Ewen PhD DIC MChem

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Employment

Nov 2017 - Present

Research Associate
Department of Mechanical Engineering, Imperial College London

- Investigating atomic-scale behaviour at solid-liquid interfaces using molecular simulations.
- Design and deliver interdisciplinary research projects to solve fundamental problems of high industrial importance - mostly related to tribology and lubrication science.
- Awarded prestigious 12-month *Doctoral Prize Fellowship* from the EPSRC.
- Established personal collaborations with several industrial partners (Shell, SKF, Afton Chemical) and academic institutions (ETH Zürich, Swinburne, Saarland, Modena).
- Named researcher on Royal Society *International Exchanges Grant* with Swinburne.
- Awarded 2018 *Tribology Bronze Medal* by Institution of Mechanical Engineers (IMechE).
- Awarded 2019 *Innovation in Tribology Award* by Institute of Physics (IOP).
- Appointed 'Assistant Supervisor' to four industrial PhD students (Afton, Element 6, GE, P&G).
- Published 11 papers as first or second author; citations >160, *h*-index = 7 (Google Scholar).

Jan 2016 - May 2016

Computational Scientist (Postgraduate Placement)
Shell India Markets Pvt. Ltd., Bangalore

- Transferred knowledge of molecular simulations to Computational Centre of Expertise team.
- Co-authored two papers investigating potential future lubricant additives (carbon nanoparticles) and advanced simulation methodologies.

Aug 2012 - Aug 2013

Fuels Scientist (Undergraduate Placement)
Shell Global Solutions UK, Chester

- Summarized a decade of Gas-to-Liquids (GTL) Fuel research into an accessible, 60-page 'Knowledge Guide' - used in customer engagements, policy lobbying, and commercial sales.
- Awarded *Special Recognition Award* for the Shell GTL Fuel Knowledge Guide.
- Filed two patents on GTL-containing gasoline (pending) and diesel (grant) fuel compositions
- Appointed *Shell Project Leader* on a Liquefied Natural Gas (LNG) research project with external consultancy TNO.

Jun 2010 - Sep 2010

Computational Scientist (Summer Placement)
Met Office, Exeter

- Developed more sophisticated chemical models for the reactions of pollutants in the troposphere and implemented them in the Met Office climate model (HadGEM-3).
- Authored code that is critical to a number of applications, most notably the DEFRA pollution forecasts as well as for International Panel for Climate Change (IPCC) reports.

Qualifications

Nov 2014 - Nov 2017

Doctor of Philosophy, PhD
Department of Mechanical Engineering, Imperial College London

- Performed molecular simulations of lubricants and additives to explain friction behaviour.
- Collaborative Awards in Science and Engineering (CASE) studentship co-funded by the EPSRC and the Shell University Technology Centre (UTC) for Fuels and Lubricants.
- Awarded *Margaret Fishenden Centenary Memorial Prize* for best thesis in the last five years.
- Assisted with successful EPSRC grants EP/P030211/1 and EP/N025954/1.

Oct 2010 - Aug 2014 **Master of Chemistry, MChem (with Industrial Training)**
Department of Chemistry, University of Bath

- Graduated with First-Class Honours, year averages; 76 %, 72 %, 75 %, 72 %.

Specialist Skills

- Proficient in Linux-based operating systems and several programming languages.
- Experienced user of several High Performance Computing (HPC) systems; Imperial College London (cx1, cx2, Thomas), Shell (Bangalore, Houston), Met Office (IBM Power 575).
- Provide HPC support to ten MEng students, PhD students and Research Associates.
- Expert in molecular simulation software, including; LAMMPS (molecular dynamics), Quantum Espresso, VASP (density functional theory), VMD (visualisation), MAPS (pre/post process).
- Computational laboratory demonstrator in Department of Chemistry (40 hours).
- Peer-reviewed 26 manuscripts for a range of journals; *ACS Appl. Mater. Interfaces, Nano Energy, Polymers, Adv. Mater. Interfaces, Comput. Mater. Sci., Tribol. Int.,* etc. (Publons).
- Presented research at 14 national and international conferences (including 2 invited).

Publications and Patents

Peer-Reviewed Journal Articles *****Corresponding author

1. C. Ayestarán Latorre, J. P. Ewen,***** C. Gattinoni, D. Dini. Simulating Surfactant-Iron Oxide Interfaces: From Density Functional Theory to Molecular Dynamics. *J. Phys. Chem. B* **2019**.
2. S. Echeverri Restrepo, M. C. P. van Eijk, J. P. Ewen.***** Behaviour of n-Alkanes Confined between Iron Oxide Surfaces at High Pressure and Shear Rate: A Nonequilibrium Molecular Dynamics Study. *Tribol. Int.* **2019**, 137, 420-432.
3. J. P. Ewen,***** H. Gao, M. Müser, D. Dini. Shear Heating, Flow, and Friction of Confined Molecular Fluids at High Pressure. *Phys. Chem. Chem. Phys.* **2019** 21, 5813.
4. C. Gattinoni,***** J. P. Ewen, D. Dini. Adsorption of Surfactants on α-Fe_2O_3(0001): A Density Functional Theory Study. *J. Phys. Chem. C* **2018** 122, 20817-20826.
5. J. P. Ewen,***** S. K. Kannam, B. D. Todd, D. Dini. Slip of Alkanes Confined between Surfactant Monolayers Adsorbed on Solid Surfaces. *Langmuir* **2018** 34, 3864-3873.
6. J. P. Ewen, D. M. Heyes, D. Dini.* Advances in Nonequilibrium Molecular Dynamics Simulations of Lubricants and Additives. *Friction* **2018** 6, 349-386.
7. J. P. Ewen,***** C. Gattinoni, J. Zhang, D. M. Heyes, H. A. Spikes, D. Dini. On the Effect of Confined Fluid Molecular Structure on Nonequilibrium Phase Behaviour and Friction. *Phys. Chem. Chem. Phys.* **2017** 19, 17883.
8. J. P. Ewen,***** S. Echeverri Restrepo, N. Morgan, D. Dini. Nonequilibrium Molecular Dynamics Simulations of Stearic Acid Adsorbed on Iron Surfaces with Nanoscale Roughness. *Tribol. Int.* **2017** 107, 264-273.
9. J. P. Ewen,***** C. Gattinoni, F. Thakkar, N. Morgan, H. A. Spikes, D. Dini. A Comparison of Classical Force-Fields for Molecular Dynamics Simulations. *Materials* **2016** 9, 651.
10. J. P. Ewen,***** C. Gattinoni, F. Thakkar, N. Morgan, H. A. Spikes, D. Dini. Nonequilibrium Molecular Dynamics Investigation of the Reduction in Friction and Wear by Carbon Nanoparticles between Iron Surfaces. *Tribol. Lett.* **2016** 63, 38.
11. J. P. Ewen,***** C. Gattinoni, N. Morgan, H. A. Spikes, D. Dini. Nonequilibrium Molecular Dynamics Simulations of Organic Friction Modifiers Adsorbed on Iron Oxide Surfaces. *Langmuir* **2016** 32, 4450-4463.

Patents

1. R. H. Clark, J. P. Ewen, R. J. Heins, P. A. Stevenson. Fuel Composition. EP3337877A1, **2018** (Pending).
2. R. H. Clark, J. P. Ewen, R. W. M. Wardle, B. Chinnusammy, P. A. Stevenson. High Power Fuel Compositions. EP3022278B1, **2018** (Granted).