James P. Ewen PhD DIC MChem

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Employment

Oct 2020 - Present
RAEng Research Fellow
Department of Mechanical Engineering, Imperial College London

- Awarded five-years of funding (£0.5M) from the Royal Academy of Engineering (RAEng) for the project 'Controlling Friction through Molecular Engineering'.

Oct 2019 - Oct 2020
Technical Consultant
Imperial Consultants (ICON)

- Worked with NextMol and Repsol to develop virtual screening tools for lubricant development.

Oct 2017 - Oct 2020
Research Associate
Department of Mechanical Engineering, Imperial College London

- Named researcher on Engineering and Physical Sciences Research Council (EPSRC) grants.
- Designed and delivered interdisciplinary research projects to solve important fundamental problems of high industrial importance; mostly related to tribology and lubrication science.
- Established personal collaborations with industrial (Shell, SKF, Afton Chemical, Baker Hughes, P&G) and academic (ETH Zürich [Materials], Swinburne [Mathematics], Saarland [Materials], Bologna [Physics], TU Delft [Engineering], UC Merced [Engineering]) researchers.
- Collaborated with experimentalists at Imperial to validate simulations and guide experiments.

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

- Produced over a dozen technical reports, slide-packs, patents, and presentations on natural gas-based alternative fuels Gas-to-Liquids (GTL) and Liquefied Natural Gas (LNG).
- Summarized over a decade of research into an accessible, 60-page *Shell GTL Fuel Knowledge Guide* - used in customer engagements, policy lobbying, and commercial sales.
- Appointed *Shell Project Leader* on research project with external consultancy TNO.

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.
- Industrial Collaborative Awards in Science and Engineering (iCASE) studentship co-funded by the EPSRC and Shell in the Tribology Group.

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%.

Grants, Funding, and Awards

Year	Source	Grant/Funding	Value	Involvement	Project Code
2021	Imperial College London	Doctoral Training Partnership (DTP)	~£100,000	Principal Investigator (PI)	InfoEd
2021	CECAM	Web Seminar Series on Tribology (WeSST)2	£1,500	Co-Organiser (with Chiara Gattinoni)	n/a
2020	Royal Academy of Engineering	Research Fellowship	£500,000	PI	n/a
2020	RSC, IoP, IMechE	WeSST1	£2,500	Co-Organiser (with Chiara Gattinoni)	n/a
2019	EPSRC (UK Fluids Network)	Special Interest Group in Non-Equilibrium Molecular Dynamics	£2,000	Co-Leader (with Edward Smith)	n/a
2019	Jost Fund	Travel Grant	£1,400	Awardee	n/a
2018	Royal Society	International Exchanges Grant	£12,000	Named Researcher	IES\R3\170233
2017	EPSRC	Doctoral Prize Fellowship	£51,426	Awardee	EP/R513052/1
Total as PI			**£670,826**		
2021	EPSRC	Prosperity Partnership (InFUSE)	£4,191,430	Assistant Supervisor (AS) and proposal writing	EP/V038044/1
2020	P&G/EPSRC	PhD Funding	~£100,000	AS and proposal writing	InfoEd
2019	Baker Hughes	PhD Funding	~£100,000	AS and proposal writing	InfoEd P81205
2017	Afton Chemical/ EPSRC	PhD Funding	~£100,000	AS and proposal writing	InfoEd P71019
2017	EPSRC	Grant (PI – Spikes)	£578,903	Proposal writing	EP/P030211/1
2016	EPSRC	Established Career Fellowship (PI – Dini)	£1,205,326	Proposal writing	EP/N025954/1

Year	Source	Award	Significance
2019	IoP	Innovation in Tribology	Award and invited lecture at Institute of Physics
2019	IoP	Best Poster Prize	Presented at Institute of Physics Tribology Fair
2019	Imperial College	President's Award for Outstanding AS	Departmental nominee, commended for effective support and feedback
2018	IMechE	Tribology Bronze Medal	For showing excellent promise in the field of tribology (one awarded per year)
2018	Imperial College	Margaret Fishenden Centenary Memorial Prize	Best PhD thesis in the Department of Mechanical Engineering over the previous five year period
2017	Elsevier	Certificate of Outstanding Contribution to Reviewing	Outstanding reviewer for; *Comput. Mater. Sci., Surf. Coat. Tech*., and *Tribol. Int*.
2016	IMechE	Best Presentation Prize	Presented at 25th IMechE Mission of Tribology

2013	Shell	Special Recognition Award	For outstanding contribution to the GTL Fuel Knowledge Guide
2013	Shell	Inventor Recognition Award	For two fuel formulation patents

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Esteem Indicators

- Published 22 papers as major contributing author; citations >450, *h*-index = 11 (Scholar).
- Affiliate of the Institute of Molecular Science and Engineering (IMSE), Energy Futures Lab (EFL), and Thomas Young Centre (TYC).
- Member of the Early Career Editorial Board of *Tribology Letters* (Springer Nature).
- Peer-reviewed >50 manuscripts for a range of journals including; *ACS Appl. Mater. Interfaces, Polymers, Adv. Mater. Interfaces, Comput. Mater. Sci., Tribol. Int., Tribol. Lett.*, etc. (Publons).
- Experienced user of several High Performance Computing (HPC) systems; Imperial College London (cx1, cx2, Thomas, Young), Shell (Bangalore, Houston), Met Office (IBM Power 575).
- Expert in molecular simulation software, including; LAMMPS (molecular dynamics), Quantum Espresso, VASP (density functional theory), VMD (visualisation), MAPS (pre/post process).
- Co-authored most cited paper of 2018 in the open access journal *Friction* (Springer Nature).
- Co-organised CECAM workshop and UK Fluid Network NEMD SIG meetings.

Teaching and Supervision

- Provide regular HPC support to more than ten master's students, PhD students and PDRAs.
- Marker for ME3 and ME4 Project Reports in Department of Mechanical Engineering.
- Computational laboratory demonstrator in Department of Chemistry (40 hours).
- *Assistant Supervisor* to seven industry and/or UKRI-funded PhD students (one graduated):

1. Egheosa Ogbomo (2021-2025) – funded by DTP from Department of Mechanical Engineering
2. Muhammad Rizwanur Rahman (2021-2025) – funded by Shell & Beit Scholarship
3. Erik Weiand (2020-2024) – funded by P&G & EPSRC (iCASE)
4. Jagjeevan S. Bhamra (2019-2023) – funded by Baker Hughes
5. Amran Mohamed (2019-2023) – funded by Shell & SSCP-DTP
6. Mohamed Abdelbar (2018-2022) – funded by TSM-CDT
7. Carlos Ayestarán Latorre (2017-2021) – funded by Afton Chemical & TSM-CDT
8. Branislav Dzepina (2016-2020) – funded by Element Six & DST-CDT (graduated).

Publications and Patents

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

1. J.S. Bhamra, J.P. Ewen,***** C. Ayestarán Latorre, J.A.R. Bomidi, M.W. Bird, N. Dasgupta, A.C.T. van Duin, D. Dini. Interfacial Bonding Controls Friction in Diamond–Rock Contacts. *J. Phys. Chem. C.* **2021** 125, 18395-18408.
2. T. Reddyhoff, J.P. Ewen,***** P. Deshpande, M. Frogley, M.D. Welch, W. Montgomery. Macroscale Superlubricity and Polymorphism of Long-Chain n-Alcohols. *ACS Appl. Mater. Interfaces.* **2021** 13, 9239-9251.
3. H. Gao, J.P. Ewen,***** R. Hartkamp, M.H. Müser, D. Dini. Scale-Dependent Friction–Coverage Relations and Non-Local Dissipation in Surfactant Monolayers. *Langmuir*. **2021** 37, 2406-2418.
4. J.P. Ewen,* H. Spikes, D. Dini. Contributions of Molecular Dynamics Simulations to Elastohydrodynamic Lubrication. *Tribol. Lett.* **2021** 69**,** 24.
5. C. Ayestarán Latorre,* J.P. Ewen, D. Dini, M.C. Righi. Ab Initio Insights into the Interaction Mechanisms between Boron, Nitrogen and Oxygen Doped Diamond Surfaces and Water Molecules. *Carbon* **2021** 171, 575-584.

6. N.D. Kondratyuk, V.V. Pisarev, J.P. Ewen.* Probing the High-Pressure Viscosity of Hydrocarbon Mixtures using Molecular Dynamics Simulations. *J. Chem. Phys.* **2020** 153, 154502.
7. Z. Tan, J.P. Ewen, S. Galvan, A.E. Forte, E. De Momi, F. Rodriguez y Baena, D. Dini. What Does a Brain Feel Like? *J. Chem. Educ.* **2020** 97, 4078-4083.
8. J.P. Ewen,***** C. Ayestarán Latorre, C. Gattinoni, A. Khajeh, J.D. Moore, J.E. Remias, A. Martini, D. Dini. Substituent Effects on the Thermal Decomposition of Phosphate Esters on Ferrous Surfaces. *J. Phys. Chem. C* **2020** 124, 9852-9865.
9. J. Zhang, J.P. Ewen, M. Ueda, J.S.S. Wong, H.A. Spikes.***** Mechanochemistry of Zinc Dialkyldithiophosphate on Steel Surfaces under Elastohydrodynamic Lubrication Conditions. *ACS Appl. Mater. Interfaces* **2020** 12, 6662-6676.
10. 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**, 123, 6870-6881.
11. 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.
12. J.P. Ewen,***** H. Gao, M.H. Müser, D. Dini. Shear Heating, Flow, and Friction of Confined Molecular Fluids at High Pressure. *Phys. Chem. Chem. Phys.* **2019** 21, 5813.
13. 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.
14. 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.
15. J.P. Ewen, D.M. Heyes, D. Dini.* Advances in Nonequilibrium Molecular Dynamics Simulations of Lubricants and Additives. *Friction* **2018** 6, 349-386.
16. 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.
17. 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.
18. J.P. Ewen,***** C. Gattinoni, F. Thakkar, N. Morgan, H.A. Spikes, D. Dini. A Comparison of Classical Force-Fields for Molecular Dynamics Simulations of Lubricants. *Materials* **2016** 9, 651.
19. 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.
20. 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.

Preprint

1. C. Ayestarán Latorre, J.E. Remias, J.D. Moore, H.A. Spikes, D. Dini, J.P. Ewen.***** Mechanochemistry of Phosphate Esters Confined between Sliding Iron Surfaces. *Research Square Preprint* **2021**.

Book Chapter ***** = Corresponding author

1. J.P. Ewen, E. Ramos Fernández, E.R. Smith, D. Dini.* Nonequilibrium Molecular Dynamics Simulations of Tribological Systems. In: M. Paggi, D. Hills (eds.), Modeling and Simulation of Tribological Problems in Technology, *CISM, Springer*, 95-130, **2020**.

Granted Patents

1. R.H. Clark, J.P. Ewen, R.J. Heins, P.A. Stevenson. Fuel Composition. EP3337877B1. **2018**.
2. R.H. Clark, J.P. Ewen, R.W.M. Wardle, B. Chinnusammy, P.A. Stevenson. High Power Fuel Compositions. EP3022278B1, **2018**.

Conference Presentations and Invited Talks

1. J.P. Ewen, Mechanochemistry of Lubricant Additives: Tribometer Experiments and Molecular Simulations. *Nanolubrication Conference, Durham University.* **2021**.[+]
2. J.P. Ewen, Macroscale Superlubricity and Polymorphism of Long-Chain n-Alcohols. *Webinar, Shell.* **2021**.[+]
3. J.P. Ewen, Macroscale Superlubricity and Polymorphism of Long-Chain n-Alcohols. *Webinar, Klueber Lubrication.* **2021**.[+]
4. J.P. Ewen, Molecular Simulations of Tribological Systems using MAPS and LAMMPS. *Webinar, Scienomics SARL.* **2021**.[+]
5. J.P. Ewen and Daniele Dini, Virtual Experiments in Tribology. *Webinar, Surface Ventures.* **2021**.[+]
6. J.P. Ewen, The Role of Tribology in Achieving Net-Zero Emissions from Transportation. *Webinar, Condensed Matter Physics Institute, University of York.* **2021**.[+]
7. J.P. Ewen, Molecular Dynamics Simulations in Tribology. *Webinar, Joint Institute for High Temperatures, Russian Academy of Sciences.* **2021**.[+]
8. J.P. Ewen, Meet the experts panel session member on 'Tribochemistry and Film Formation'. *STLE Tribology Frontiers, Online* **2020**.[+]
9. J.P. Ewen, T. Reddyhoff, H.A. Spikes, D. Dini. Molecules under Pressure. (Spotlight Presentation) *STLE Tribology Frontiers, Online* **2020**.[+]
10. J.P. Ewen, J. Zhang, H.A. Spikes. Mechanochemistry of tribofilm formation. *Molecular Mechanisms of Tribochemistry and Lubrication, CECAM, Switzerland* **2020**.[+]
11. J.P. Ewen, NEMD in Tribology. *UK Fluids Network Special Interest Group Meeting on NEMD, Brunel University* **2020**.
12. J.P. Ewen, Small is big in tribology. *Institute of Physics Winter Tribology Fair, Sheffield, UK* **2020** (Innovation in Tribology Award).[+]
13. J.P. Ewen, D. Dini. Modelling of tribological contacts from first principles. *International Tribology Conference, Sendai, Japan* **2019**.
14. J.P. Ewen, Multiscale Modelling in Tribology. *Institute of Physics Winter Tribology Fair, London, UK* **2018** (Poster).
15. J.P. Ewen, S.K. Kannam, B.D. Todd, D. Dini. Slip of Hexadecane on Organic Friction Modifier Monolayers, *APS March Meeting, Los Angeles, USA* **2018**.
16. J.P. Ewen, H.A. Spikes, D. Dini. Effect of Confined Fluid Molecular Structure on Nonequilibrium Phase Behaviour and Friction. *21st International Colloquium on Tribology, Technische Akademie Esslingen, Germany* **2018**.
17. J.P. Ewen, H.A. Spikes, D. Dini. Effect of Confined Fluid Molecular Structure on Nonequilibrium Phase Behaviour and Friction. *6th World Tribology Congress, Beijing, China* **2017**.
18. J.P. Ewen, Molecular Modelling of Lubricants and Additives. *IMechE Tribology Modelling, Birmingham, UK* **2017**.[+]
19. J.P. Ewen, C. Gattinoni, N. Morgan, H. A. Spikes, D. Dini. Nonequilibrium Molecular Dynamics Simulations of Friction Modifier Additives. *ACS Spring Meeting, San Francisco, USA* **2017**.
20. J.P. Ewen, Molecular Dynamics Simulations of Lubricants and Additives. *25th IMechE Mission of Tribology, London, UK* **2016**.

21. J.P. Ewen, C. Gattinoni, F. Thakkar, N. Morgan, H. A. Spikes, D. Dini. Molecular Dynamics Investigation of the Reduction in Friction and Wear by Carbon Nanoparticles. *STLE Tribology Frontiers, Chicago, USA* **2016**.
22. J.P. Ewen, Molecular Dynamics Simulations of Lubricants and Additives. *Shell Research UK*, *London, UK* **2016**.[+]
23. J.P. Ewen, C. Gattinoni, N. Morgan, H. A. Spikes, D. Dini. Nonequilibrium Molecular Dynamics Simulations of Organic Friction Modifiers. *STLE Annual Meeting, Las Vegas, USA* **2016**.
24. J.P. Ewen, C. Gattinoni, N. Morgan, D. Dini. Force-Field Selection for Molecular Dynamics Simulations of Lubricants and Additives. *20th International Colloquium on Tribology, Technische Akademie Esslingen, Germany* **2016**.[+]
25. J.P. Ewen, Molecular Dynamics Simulations of Lubricants and Additives. *Shell Technology Centre Bangalore, India* **2016**.[+]
26. J.P. Ewen, C. Gattinoni, N. Morgan, H. A. Spikes, D. Dini. Molecular Dynamics Investigation of the Atomic-Scale Behaviour of Organic Friction Modifiers. *STLE Tribology Frontiers, Denver, USA* **2015**.

[+] = Invited talk