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EDUCATION

University of Cambridge (Advisor: Prof. David Fairen-Jimenez) Cambridge, UK

Ph.D. in Chemical Engineering *Sept 2019 - Present*

University of California, Berkeley (Advisor: Prof. Berend Smit) Berkeley, CA

Master of Science in Chemical Engineering; GPA: 3.976/4 *Aug. 2016 – May 2017*

Manipal Institute of Technology Manipal, India

Bachelor of Technology in Chemical Engineering; GPA: 8.91/10 *Jul. 2011 – May 2015*

PUBLICATIONS (⊥ denotes equal contribution, * denotes corresponding author)

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1. Xianhui Tang, Hong Jiang, Yubing Si, Nakul Rampal, Wei Gong, Cheng Cheng, Xing Kang, David Fairen-Jimenez, Yong Cui, Yan Liu*. Endohedral functionalization of chiral metal-organic cages for encapsulating achiral dyes to induce circularly polarized luminescence, **Chem**, 2021

2. Nakul Rampal⊥, Abdulmalik Ajenifuja⊥, Andi Tao⊥, Christopher Balzer, Matthew S. Cummings, Arwyn Evans, Rocio Bueno-Perez, David J. Law, Camille Petit, Flor Siperstein, Martin P. Attfield, Megan Jobson, Peyman Z. Moghadam, David Fairen-Jimenez*. The development of a comprehensive toolbox based on multi-level, high-throughput screening of MOFs for CO/N_2 separations, **Chemical Science**, 2021

3. Xu Chen, Yunhui Zhang, Nakul Rampal, Rachel Hewitt, Giorgio Divitini, Christopher A O'Keefe, Xiewen Liu, Daniel J Whitaker, John W Wills, Ravin Jugdaosingh, Jonathan J Powell, Han Yu*, Clare P Grey, Oren A Scherman, David Fairen-Jimenez*. Formulation of Metal-Organic Framework-Based Drug Carriers by Controlled Coordination of Methoxy PEG Phosphate: Boosting Colloidal Stability and Redispersibility, **Journal of the American Chemical Society**, 2021, 143(34), 12557-13572 (Work highlighted in C&EN and is also on the cover of Volume 143, Issue 34 of the Journal of the American Chemical Society)

4. David Madden, Robin Babu, Ceren Camur, Nakul Rampal, Joaquin Silvestre-Albero, Teresa Curtin, David Fairen-Jimenez*. Monolithic metal-organic frameworks for carbon dioxide separation, **Faraday Discussions**, 2021

5. Bablu Meghwal, Nakul Rampal, Ateeque Malani*, Investigation of Adhesion between Heavy oil/Bitumen and Reservoir Rock: A Molecular Dynamics Study, **Energy & Fuels**, 2020, 34(12), 16023-16034

6. Kathryn S. Deeg, Daiane Damasceno Borges, Daniele Ongari, Nakul Rampal, Leopold Talirz, Aliaksandr V. Yakutovich, Johanna M. Huck, Berend Smit*. In Silico Discovery of Covalent Organic Frameworks for Carbon Capture, **ACS Applied Materials & Interfaces,** 2020, 12, 19, 21559-21568

7. Sudi Jawahery, Nakul Rampal, Seyed Mohamad Moosavi, Mathew Witman, Berend Smit*. *Ab Initio* Flexible Force Field Development for Metal-Organic Frameworks Using Non-Bonded Dummy Models to Describe Coordination Bonds, **Journal of Chemical Theory and Computation**, 2019, 15, 6, 3666-3677

8. Meena B. Singh, Nakul Rampal, Ateeque Malani*. Structural Behavior of Isolated Asphaltene Molecules at the Oil-Water Interface, **Energy & Fuels**, 2018, 32(8), 8259-8267

PREPRINTS (⊥ denotes equal contribution, * denotes corresponding author)

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1. Johannes Osterrieth, James Rampersad, David G Madden, Nakul Rampal, Luka Skoric, Bethany Connolly, Mark Allendorf, Vitalie Stavila, Jonathan Snider, Rob Ameloot, Joao Marreiros, Conchi O Ania, Diana CS Azevedo, Enrique Vilarrasa-García, Bianca F Santos, Xian-He Bu, Xe Zang, Hana Bunzen, Neil Champness, Sarah L Griffin, Banglin Chen, Rui-Biao Lin, Benoit Coasne, Seth M Cohen, Jessica C Moreton, Yamil J Colon, Linjiang Chen, Rob Clowes, François-Xavier Coudert, Yong Cui, Bang Hou, Deanna D'Alessandro, Patrick W Doheny, Mircea Dinca, Chenyue Sun, Christian Doonan, Michael Huxley, Jack D Evans, Raffaele Ricco, Omar K Farha, Karam B Idrees, Timur Islamoglu, Pingyun Feng, Huajun Yang, Ross Forgan, Dominic Bara, Shuhei Furukawa, Elisabeth Sanchez, Jorge Gascon, Selvedin Telalovic, Sujit K Ghosha, Soumya Mukherjee, Matthew R Hill, Muhammad Munir Sadiq, Patricia Horcajada, Pablo Salcedo-Abraira, Katsumi Kaneko, Radovan Kukobat, Jeffrey Kenvin, Seda Keskin, Susumu Kitagawa, Kenichi Otake, Ryan P Lively, Stephen JA DeWitt, Philip L Llewellyn, Bettina Lotsch, Sebastian T Emmerling, Alexander Pütz, Carlos Martí-Gastaldo, Natalia Muñoz, Javier Garcia-Martinez, Noemi Linares, Daniel Maspoch, Jose Antonio Suarez, Peyman Moghadam, Rama Oktavian, Russell Morris, Paul Wheatley, Jorge Navarro, Camille Petit, David Danaci, Matthew Rosseinsky, Alexandros Katsoulidis, Martin Schroder, Xue Han, Sihai Yang, Christian Serre, Georges Mouchaham, David Sholl, Raghuram Thyagarajan, Daniel Siderius, Randall Q Snurr, Rebecca B Goncalves, Shane G Telfer, Seok J Lee, Valeska Ting, Jemma Rowlandson, Takeshi Uemura, Tomoya Iiyuka, Monique van der Veen, Davide Rega, Veronique Vanspeybroeck, Aran Lamaire, Sven Rogge, Krista Walton, Lukas W Bingel, Stefan Wuttke, Jacopo Andreo, Omar Yaghi, Bing Zhang, Cafer Yavuz, Thien Nguyen, Felix Zamora, Carmen Montoro, Hong-Cai Zhou, Kirchon Angelo, David Fairen-Jimenez*. How reproducible are Surface Areas Calculated from the BET Equation? **ChemRxiv**, 2021

2. Mark Carrington⊥, Nakul Rampal⊥, David G Madden, Daniel O'Nolan, Nicola Pietro Maria Casati, Giorgio Divitini, Ritums Cepitis, Jesus A Martin Ilan, Ceren Camur, Joaquin Silvestre-Albero, Felix Zamora, Sergei Taraskin, Karena W Chapman, David Fairen-Jimenez*. Sol-Gel Processing of a Covalent Organic Famework for the Generation of Hierarchically Porous Monolithic Adsorbents, **ChemRxiv**, 2021

INVITED TALKS/PRESENTATIONS

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1. Presentation (virtual) at the 2nd International School on Porous Materials: MOFschool2021, Lake Como School of Advanced Studies, 21-25 June 2021
2. Presentation (virtual) at the bp-ICAM Annual Conference 2020, 20th-21st October 2020
3. Invited talk at Chalmers University of Technology (Department of Physics), 4th February 2019.
4. Invited talk at Karlsruhe Institute of Technology (Department of Theoretical Chemical Biology), 1st February 2019.
5. Invited talk at the Theoretical Chemistry Seminar at the Norwegian University of Science and Technology (NTNU), 14th December 2018.

EXPERIENCE

Smit Group Berkeley, CA

Researcher *March 2017 – July 2019*

- Studying the deformation of IRMOF-74 using Hybrid MC/MD techniques and umbrella sampling.
- Built an analytical model to calculate the Henry coefficient in different pore geometries.
- Modified RASPA, to perform calculations in the Osmotic Ensemble.
- Built a plug-in for AiiDA to calculate the parasitic energy.

University of California, Berkeley Berkeley, CA

Graduate Student Instructor *Jan 2017 – May 2017*

-Graded Homework and held weekly discussion sessions for the course Mathematical Methods in Geophysics.

- Topics taught include vector calculus, elastic stress/strain relations, fluid mechanics, thermodynamics, partial differential equations, Fourier analysis and contour integrals.
- Nominated for the **Outstanding GSI Award**.

AWARDS

- Cambridge International Scholarship
- Trinity Henry-Barlow Scholarship (Honorary)
- Merit based Scholarship in Fall 2016 and Spring 2017 at UC, Berkeley
- Top 3 of the graduating class at MIT, Manipal
- School Topper Medal in the Unified Cyber Olympiad
- School Wiz Kid Medal in the 10th National Science Olympiad
- 1 of 3 winners of the Global Young Scientists Summit 2021 video competition
- Full bursary to attend MOFSchool2021 provided by the Italian Crystallographic Association