Nakul Rampal

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Experience

University of California, Berkeley Berkeley, CA
Postdoctoral Scholar; BIDMaP Fellow
Advisors: Prof. Omar Yaghi, Dean Jennifer Chayes, Prof. Christian Borgs Jun 2023 – Present

Education

University of Cambridge Cambridge, UK
Ph.D. in Chemical Engineering
Advisor: Prof. David Fairen-Jimenez, Cambridge Trust Scholar Sep 2019 – Jul 2023

University of California, Berkeley Berkeley, CA
M.S. in Chemical Engineering; GPA: 3.976/4
Advisor: Prof. Berend Smit, Merit-based Scholarship Aug 2016 – May 2017

Manipal Institute of Technology Manipal, India
B.Tech. in Chemical Engineering; GPA: 8.91/10
Thesis with Prof. Ateeque Malani (IIT Bombay) Jul 2011 – May 2015

Teaching

- Graduate Student Instructor for ”Mathematical Methods in Geophysics”, Spring 2017, University of California, Berkeley (Nominated for the Outstanding GSI Award)
- Supervisor for the module on ”Adsorption and Advanced Nanoporous Materials”, Chemical Engineering Tripos, Michaelmas Term 2022, University of Cambridge
- Co-instructor (6-week summer course) on ”Adsorption and Nanoporous Materials” run by Cambridge Enterprise — Summer 2021 (1 course), 2022 (2 courses), 2023 (1 course)
- Guest instructor for the course *PHYS H190 Physical Systems by and for Artificial Intelligence*, Spring 2025, University of California, Berkeley
- Guest instructor for *CHEM 96 - Introduction to Research and Study*, College of Chemistry, Fall 2024, University of California, Berkeley

Mentorship

- Mythili Sutharson, MPhil in Advanced Chemical Engineering, Oct 2019 – Aug 2020 — Currently Associate Consultant at Bain
- Hiu Ki Wong, Part IIB in Chemical Engineering, Oct 2020 – Apr 2021 — Currently Data Engineer at Pirical
- George Irving, Part IIB in Chemical Engineering, Oct 2021 – Apr 2022 — Awarded 1st prize for best poster presentation
- Khalid Al-Otaibi, MPhil in Advanced Chemical Engineering, Apr 2022 – Aug 2022 (Saudi Aramco)
- Zhiling Zheng, PhD in Chemistry, Jun 2023 – Dec 2023 — Currently Assistant Professor, Washington University in St. Louis

- Ali Al-Awadhi, PhD in Chemistry, Sep 2023 – Ongoing
- Kaiyu Wang, PhD in Chemistry, Sep 2023 – Ongoing
- Juri Al-Johani, BS in Electrical Engineering & Computer Science, Dec 2023 – Jun 2024
- Joe Fu, BS/PhD in Electrical Engineering & Computer Science, Jun 2024 – Ongoing
- Daniel Ahn, PhD in Chemistry, Jan 2025 – Ongoing
- Dongha Kim, B.S. in Chemical Engineering/Data Science, Jul 2025 – Ongoing
- Om Kannan, B.S. in Applied Math/Data Science, Jul 2025 – Ongoing

Awards

- Cambridge International Scholarship
- Trinity Henry-Barlow Scholarship
- Merit-based Scholarship (Fall 2016 and Spring 2017), University of California, Berkeley
- Top 3 of the graduating class, Manipal Institute of Technology
- School Topper Medal, Unified Cyber Olympiad
- School Wiz Kid Medal, 10th National Science Olympiad

Selected Publications as First Author

([§] denotes equal contribution, * denotes corresponding author)

1. Yuang Shi[§], **Nakul Rampal**[§], Chengbin Zhao, Joe Fu, Christian Borgs, Jennifer T. Chayes, Omar Yaghi*. *Comparison of LLMs in Extracting Synthesis Conditions and Generating Q&A Datasets for Metal-Organic Frameworks*, Digital Discovery, 2025.

2. **Nakul Rampal**, Kaiyu Wang, Matthew Burigana, Lingxiang Hou, Juri Al-Johani, Anna Sackmann, Hanan S. Murayshid, Walaa A. AlSumari, Arwa M. AlAbdulkarim, Nahla E. AlHazmi, Majed O. Alawad, Christian Borgs*, Jennifer Chayes*, Omar M. Yaghi*. *Single and Multi-Hop Question-Answering Datasets for Reticular Chemistry with GPT-4-Turbo*, Journal of Chemical Theory and Computation, 2024.

3. Mark Carrington[§], **Nakul Rampal**[§], David G Madden, Daniel O'Nolan, Nicola Pietro Maria Casati, Giorgio Divitini, Ritum 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 Framework for the Generation of Hierarchically Porous Monolithic Adsorbents*, Chem, 2022.

4. David G. Madden[§]*, Daniel O'Nolan[§], **Nakul Rampal**[§], Robin Babu, Ceren Camur, Ali N. Al Shakhs, Shi-Yuan Zhang, Graham A. Rance, Javier Perez, Nicola Pietro Maria Casati, Carlos Cuadrado-Collados, Denis O'Sullivan, Nicholas P. Rice, Thomas Gennett, Philip Parilla, Sarah Shulda, Katherine E. Hurst, Vitalie Stavila, Mark D. Allendorf, Joaquin Silvestre-Albero, Alexander C. Forse, Neil R. Champness, Karena W. Chapman*, David Fairen-Jimenez*. *Densified HKUST-1 Monoliths as a Route to High Volumetric and Gravimetric Hydrogen Storage Capacity*, Journal of the American Chemical Society, 2022.

5. Johannes Osterrieth[§], James Rampersad[§], David G. Madden[§], **Nakul Rampal**[§], Luka Skoric, Bethany Connolly, Mark Allendorf, Vitalie Stavila, Jonathan Snider, Rob Ameloot, . . . , 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?*, Advanced Materials, 2022.

6. **Nakul Rampal**§, Abdulmalik Ajenifuja§, Andi Tao§, Christopher Balzer, Matthew S. Cummings, Arwyn Evans, Rocio Bueno-Perez, David J. Law, Leslie W. Bolton, 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.

Selected Publications as Contributing Author

(§ denotes equal contribution, * denotes corresponding author)

6. Zhiling Zheng, **Nakul Rampal**, Théo Jaffrelot Inizan, Christian Borgs, Jennifer Chayes, Omar Yaghi*. *Large language models for reticular chemistry*, Nature Reviews Materials, 2025.

7. Elena Avila§, Hayden Salway§, Edoardo Ruggeri, Ceren Çamur, **Nakul Rampal**, Tiarnan A. S. Doherty, Oliver D. I. Moseley, Samuel D. Stranks, David Fairen-Jimenez*, Miguel Anaya*. *Better together: Monolithic halide perovskite@metal-organic framework composites*, Matter, 2024.

8. Zhiling Zheng, Zhiguo He, Omar Khattab, **Nakul Rampal**, Matei Zaharia, Christian Borgs, Jennifer Chayes, Omar Yaghi*. *Image and Data Mining in Reticular Chemistry Powered by GPT-4V*, Digital Discovery, 2024.

9. Ali Al-Awadhi, Saumil Chheda, Gautam Stroscio, Zichao Rong, Daria Kurandina, Lac Ha Nguyen, **Nakul Rampal**, Zhiling Zheng, Laura Gagliardi, Omar Yaghi*. *Harvesting Water from Air with High-Capacity, Stable Furan-Based Metal-Organic Frameworks*, Journal of the American Chemical Society, 2024.

10. Zhiling Zheng, Ali Al-Awadhi, Saumil Chheda, Ephraim Neumann, **Nakul Rampal**, Shengchao Liu, Lac Ha Nguyen, Yen-hsu Lin, Zichao Rong, Ilja Siepmann, Laura Gagliardi, Anima Anandkumar, Christian Borgs, Jennifer Chayes, Omar Yaghi*. *Shaping the Water-Harvesting Behaviour of Metal-Organic Frameworks Aided by Fine-Tuned GPT Models*, Journal of the American Chemical Society, 2023.

11. Zhiling Zheng§, Zichao Rong§, **Nakul Rampal**, Christian Borgs, Jennifer Chayes, Omar Yaghi*. *A GPT-4 Reticular Chemist for Guiding MOF Discovery*, Angewandte Chemie, 2023.

12. Zhiling Zheng, Oufan Zhang, Lac Ha Nguyen, **Nakul Rampal**, Ali Al-Awadhi, Zichao Rong, Teresa Head-Gordon, Christian Borgs, Jennifer Chayes, Omar Yaghi*. *ChatGPT Research Group for Optimizing the Crystallinity of MOFs and COFs*, ACS Central Science, 2023.

13. Xu Chen*, Sergio Mercado Argandona, Francesca Melle, **Nakul Rampal**, David Fairen-Jimenez*. *Advances in surface functionalization of next-generation metal-organic frameworks for biomedical applications: design, strategies, and prospects*, Chem, 2023.

14. Ceren Camur, Robin Babu, Jose A. Suarez del Pino, **Nakul Rampal**, Javier Perez-Carvajal, Philipp Hugenell, Sebastian-Johannes Ernst, Joaquin Silvestre-Albero, Inhar Imaz, David G. Madden, Daniel Maspoch, David Fairen-Jimenez*. *Monolithic Zirconium-Based Metal–Organic Frameworks for Energy-Efficient Water Adsorption Applications*, Advanced Materials, 2023.

15. Xianhui Tang§, Chunlong Meng§, **Nakul Rampal**, Aurelia Li, Xu Chen, Wei Gong, Hong Jiang, David Fairen-Jimenez, Yong Cui, Yan Liu*. *Homochiral Porous Metal–Organic Polyhedra with Multiple Kinds of Vertices*, Journal of the American Chemical Society, 2023.

16. David H. Le, Ryan P. Loughan, Andrzej Gładysiak, **Nakul Rampal**, Isabelle A. Brooks, Ah-Hyung Alissa Park, David Fairen-Jimenez, Kyriakos C. Stylianou*. *Lanthanide metal–organic frameworks for the fixation of CO_2 under aqueous-rich and mixed-gas conditions*, Journal of Materials Chemistry A, 2022.

17. 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.

18. Xu Chen, Yunhui Zhang, **Nakul Rampal**, Rachel Hewitt, Giorgio Divitini, Christopher A. O'Keefe, Xiewen Liu, Daniel J. Whitaker, John W. Wills, Ravin Jugdaohsingh, 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.

19. 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.

20. Bablu Meghwal, **Nakul Rampal**, Ateeque Malani*. *Investigation of Adhesion between Heavy Oil/Bitumen and Reservoir Rock: A Molecular Dynamics Study*, Energy & Fuels, 2020.

21. 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.

22. Sudi Jawahery, **Nakul Rampal**, Seyed Mohamad Moosavi, Mathew Witman, Berend Smit*. *Ab Initio Flexible Force Field for Metal-Organic Frameworks Using Dummy Model Coordination Bonds*, Journal of Chemical Theory and Computation, 2019.

23. Meena B. Singh, **Nakul Rampal**, Ateeque Malani*. *Structural Behavior of Isolated Asphaltene Molecules at the Oil-Water Interface*, Energy & Fuels, 2018.

Preprints

(§ denotes equal contribution, * denotes corresponding author)

1. **Nakul Rampal**§, Dongrong Joe Fu§, Chengbin Zhao, Hanan S. Murayshid, Albatool A. Abaalkhail, Nahla E. Alhazmi, Majed O. Alawad, Christian Borgs*, Jennifer T. Chayes*, Omar M. Yaghi*. *An Automated Evaluation Agent for Q&A Pairs and Reticular Synthesis Conditions*, ChemRxiv, 2025.

2. Kaiyu Wang, **Nakul Rampal**, Ying Liu, Cailing Chen, Ha Nguyen, Felipe Gándara, Vivek Singh, Zichao Rong, Yuang Shi, Sebastian Neumann, Jackson Thomassian, Raynald Giovine, Punit Kumar, Robert Ritchie, Lingmei Liu, Yu Han*, Ting Xu*, Omar Yaghi*. *Fully-stretched, single-crystalline polymers of linear poly[n]catenanes*, ChemRxiv, 2025.

3. Shengchao Liu§, Weitao Du§, Yanjing Li, Zhuoxinran Li, Vignesh Bhethanabotla, **Nakul Rampal**, Omar Yaghi, Christian Borgs, Anima Anandkumar, Hongyu Guo*, Jennifer Chayes*. *A Multi-Grained Symmetric Differential Equation Model for Learning Protein-Ligand Binding Dynamics*, arXiv, 2024.

Invited Talks

1. Invited talk at the University of Milan (Department of Chemistry), 23rd June 2025.

2. Invited talk at The Chemist's Interactions – June Seminar at the University of Milan, 23rd June 2025.

3. Invited talk (virtual/in-person) at Nanyang Technological University (School of Physical and Mathematical Sciences), 21st January 2022.

4. Presentation (virtual) at the 2nd International School on Porous Materials: MOFschool2021, Lake Como School of Advanced Studies, 21-25 June 2021.

5. Presentation (virtual) at the bp-ICAM Annual Conference 2020, 20th-21st October 2020.

6. Invited talk at Chalmers University of Technology (Department of Physics), 4th February 2019.

7. Invited talk at Karlsruhe Institute of Technology (Department of Theoretical Chemical Biology), 1st February 2019.

8. Invited talk at the Theoretical Chemistry Seminar, Norwegian University of Science and Technology (NTNU), 14th December 2018.