Dr. Prabhat Prakash

Physics-informed multiscale simulation for energy storage, catalysis & aqueous chemistry

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CURRENT POSITION

Research Associate, Prof. William A. Goddard III group, California Institute of Technology **Mar 2022 – present**
DOE Fuels-from-Sunlight Hub, Liquid Sunlight Alliance (LiSA)

- Reactive machine-learned potentials for bicarbonate–carbonic acid equilibria in electrocatalysis and for lithium battery electrolytes
- Recombination reactions and ionic equilibria in water micro-environments
- Molecular modeling of photocatalysts and zeolites for carbon conversion; QM-ReaxFF studies of high-energy materials

EDUCATION

Ph.D., Physical Chemistry (Theory), IISER Pune, India (Prof. Arun Venkatnathan) **2014 – 2020**
Thesis: "Computer Simulations of CO_2 Absorption in Amino Acid Ionics & Ion Conduction in Alkali Metal Battery Electrolytes"

M.Sc., Chemistry (Physical), Banaras Hindu University, India **2012 – 2014**

B.Sc. (Hons.), Chemistry, Banaras Hindu University, India **2009 – 2012**

RESEARCH EXPERIENCE

Research Associate, IISER Pune — Na^+ battery electrolytes; CO_2 capture in methyl-piperidines **Dec 2021 – Mar 2022**

Early Career Fellow (Postdoc), IIT Gandhinagar — multiscale SEI simulations in polymer-composite electrolytes **Oct 2020 – Oct 2021**

Visiting Researcher, Temple University (Prof. Michael Zdilla) — DFT of Mn clusters; Li-ion conduction models **Jan 2020 – Jul 2020**

Fulbright–Nehru Doctoral Researcher, Temple University — experiment + theory of Li^+ migration in soft-solid electrolytes **Aug 2018 – May 2019**

NEW PREPRINT

arXiv 2611.04121 (2026). **P. Prakash**, K. Ranka, F. A. Houle, W. A. Goddard III. Bicarbonate/carbonic acid equilibria in aqueous solutions: conformational dynamics, ion-pair speciation, and free energy landscapes from ab initio molecular dynamics and metadynamics.

SELECTED PUBLICATIONS (10 OF 28)

28 published or accepted, 2 under review · h-index 11, 400+ citations · 10 as first/equal-first author (†), 6 as corresponding author (*).

1. ***Nature Materials*** 2023, 22, 627–635. **P. Prakash**, B. Fall, J. Aguirre, L. A. Sonnenberg, P. R. Chinnam, S. Chereddy, D. A. Dikin, A. Venkatnathan, S. L. Wunder, M. J. Zdilla. A soft co-crystalline solid electrolyte for lithium-ion batteries.
2. ***J. Am. Chem. Soc.*** 2026, 10.1021/jacs.6c17476. S. Goel, T. Das, **P. Prakash**, W. A. Goddard III. Mechanisms of Ammonia Synthesis over Ru Low- and High-Index Surfaces Based on Density Functional Theory Calculations.
3. ***J. Am. Chem. Soc.*** 2025, 147, 6583–6593. S. Kwon†, **P. Prakash**†, Y. Cao, F. A. Houle, W. A. Goddard III. Recombination of autodissociated water ions in a nanoscale pure water droplet.
4. ***Chemical Science*** 2021, 12, 5574–5581. **P. Prakash**, A. Shylendran, B. Fall, M. J. Zdilla, S. L. Wunder, A. Venkatnathan. Solvate sponge crystals of $(DMF)_3NaClO_4$: reversible pressure/temperature controlled juicing in a melt/press-castable sodium-ion conductor.
5. ***Materials Horizons*** 2025, 12, 10728–10739. S. C. Paul, W. A. Goddard III, M. J. Zdilla, **P. Prakash***, S. L. Wunder. Grain boundary tuning determines iodide and lithium-ion migration in a solid adiponitrile–LiI molecular crystal electrolyte.
6. ***Applied Catalysis B: Environment and Energy*** 2026, 399, 127142. C. B. Hiragond†, **P. Prakash**†, T. Das, N. S. Powar, E. Gong, J. Lee, J.-W. Jung, C.-H. Cho, W. A. Goddard III, S.-I. In. Highly selective CO_2-to-CH_4 conversion via multisun-assisted photocatalysis enabled by dual cocatalyst interfaces.

7. ***ACS Materials Letters*** 2026, 8, 764–771. S. C. Paul, W. A. Goddard III, M. J. Zdilla, **P. Prakash***, S. L. Wunder. Nanoconfined grain boundaries increase the conductivity of polycrystalline molecular crystals.
8. ***J. Mater. Chem. A*** 2018, 6, 4394–4404. **P. Prakash**, J. Aguirre, M. M. Van Vliet, P. R. Chinnam, D. A. Dikin, M. J. Zdilla, S. L. Wunder, A. Venkatnathan. Unravelling the structural and dynamical complexity of the equilibrium liquid grain-binding layer in highly conductive organic crystalline electrolytes.
9. ***ACS Applied Energy Materials*** 2026, 9, 2902–2911. V. Thakur, **P. Prakash***, R. Ranganathan. How individual versus shared coordination governs the degree of correlation in rotational versus residence times in a high-viscosity lithium electrolyte.
10. ***ChemPhysChem*** 2026, 27, e202500917 (invited). V. Thakur, **P. Prakash***, R. Ranganathan. Understanding electrolyte decomposition and interphase formation at Li metal anode in glyme-based electrolytes via DFT-MD simulations.

Full list: ppt-2.github.io · Google Scholar · ORCID

TEACHING

Co-instructor, Ch121a – Atomic-Level Simulations of Materials and Molecules, Caltech (with Prof. W. A. Goddard III) — delivered half the lectures and redesigned the course incl. periodic DFT (github.com/ppt-2/Ch121a_2026) **Spring 2026**

Guest lecturer, Ch121a, Caltech — "Simulating the molecules of life"; "Unveiling the dance of H_2O molecules" **2024, 2025**

Teaching Assistant, IISER Pune — Quantum Chemistry; Molecular Modeling & Simulation (lab curriculum design); Chemical Principles **2015 – 2017**

MENTORING

- Graduate students: Chi Zhang (Caltech; *Science Advances* 2026), Biyuan Liu (Caltech visiting; *ACS Catalysis* 2026), Vinay Thakur (IIT Gandhinagar; *ACS Appl. Energy Mater.* & *ChemPhysChem* 2026), Rohit Srikanth (Caltech), Marie E. Nikolov (Temple)
- High-school/undergraduate students: Shrish Goel (Caltech; *JACS* 2026 accepted)

GRANTS, AWARDS & FELLOWSHIPS

- Junior researcher on the joint proposal for the Liquid Sunlight Alliance, U.S. DOE Office of Basic Energy Sciences Fuels-from-Sunlight Hub
- Co-recipient, DST National Supercomputing Mission grant (DST/NSM/R&D_HPC_Applications/2021/30), India
- Fulbright–Nehru Doctoral Research Fellowship, U.S. Department of State (2018 – 2019)
- INSPIRE Fellowship, DST India — top 0.1% of high-school students nationally (2009 – 2014)

SELECTED TALKS

- **MRS Fall Meeting 2026** (upcoming), Boston — Meet the New Faculty Candidates: "Physics-Informed Multiscale Materials Modeling of Energy Storage and Conversion"; plus two orals and one poster
- **AIChE Annual Meeting 2026**, Minneapolis — Meet the Faculty and Post-Doc Candidates: "From Electrons to Electrolytes: Multiscale, Physics-Informed Simulations for Next-Generation Energy Conversion and Storage Materials"
- Invited masterclass, APS SCCM 2025, Washington DC — "Data Science for Shock and Compression"
- Invited talks: IIT Delhi (2025); Temple University (2025); University of Alabama, Huntsville (2025); InCoMACS Lucknow (2024); IIT Gandhinagar (2023); CSIR-NCL Pune (2023)
- Contributed: ACS National Meetings (2021, 2023, 2025); NERSC Annual Meeting, LBNL (2023); LiSA All-Hands (2024)

SERVICE & OUTREACH

- **Journal peer reviewer:** *Energy & Environmental Science* (RSC), *Journal of Power Sources* (Elsevier), *ACS Omega* (ACS), *RSC Advances* (RSC), *Journal of Energetic Materials* (Taylor & Francis), *Journal of Molecular Modeling* (Springer Nature)
- Lead organizer, Caltech Postdocs Launch seminar series (Spring & Fall 2024; 20 speakers)
- Fulbright ambassador, Philadelphia region (2018 – 2019); research-integrity talk and PhD panel, IISER Pune (2019)

References available on request.