Infographic Images of Condensed Phase and Interfacial Molecular Science

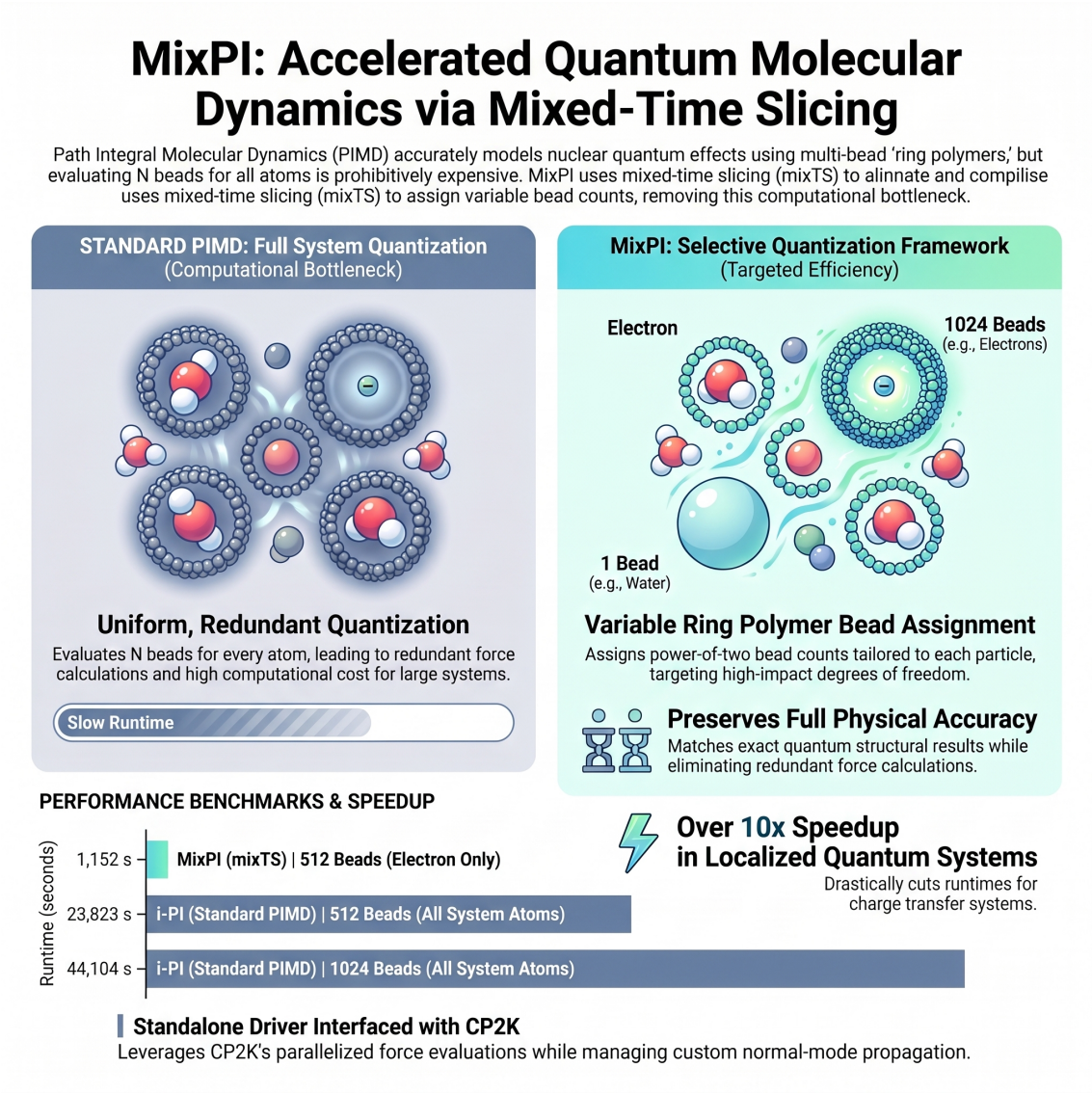
Molecular Theory and Modeling, FWP 16249

Publications (2024–2026)

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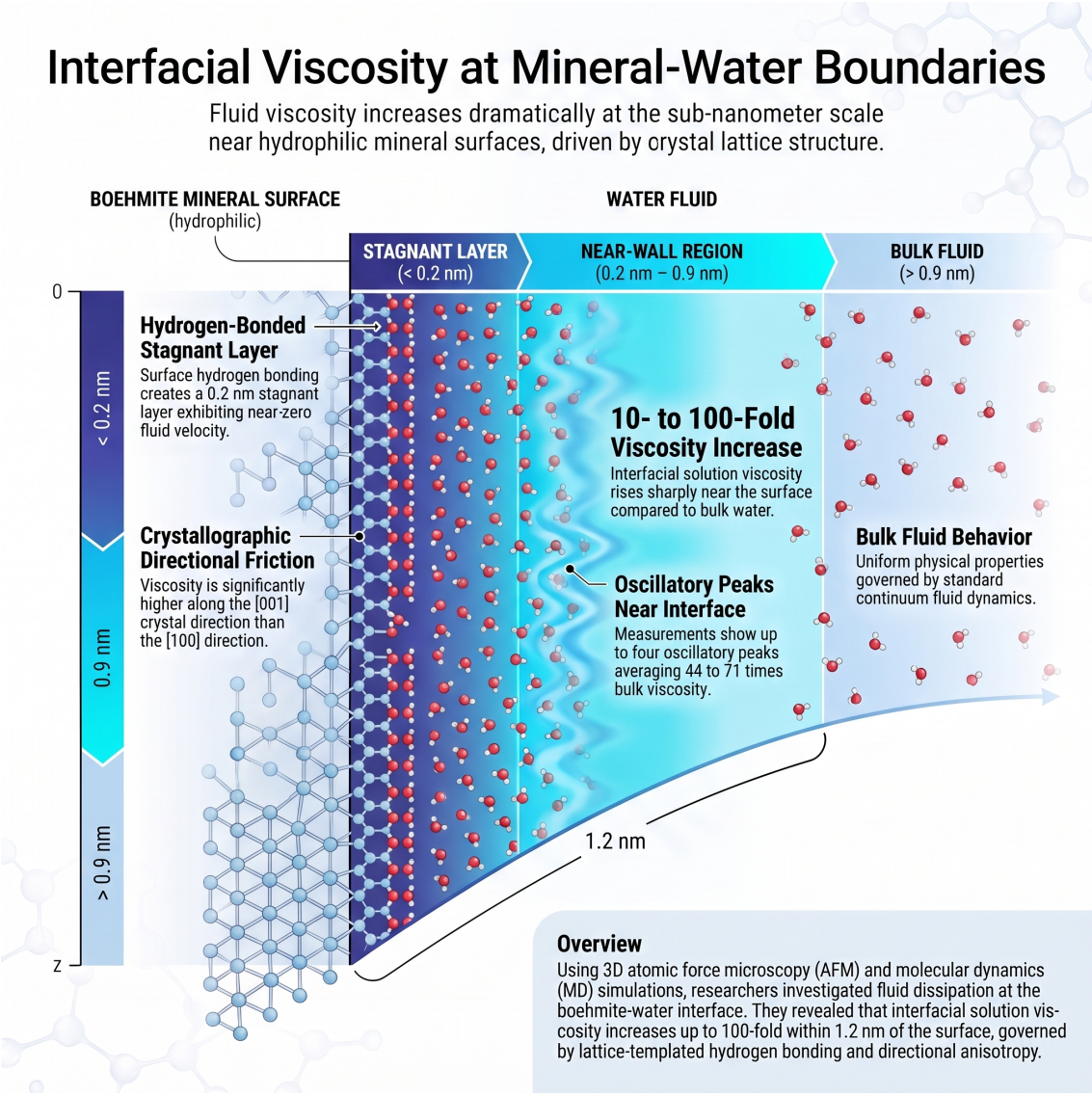
Infographics were created using Gemini Notebook from a single source PDF file of the publication and reviewed by a subject matter expert for accuracy. High level descriptions are correct. Minor details in representation may be incorrect. (Some molecules are distorted.)



MixPI: Mixed-time slicing path integral software for quantized molecular dynamics simulations

Britta A. Johnson, Siyu Bu, Christopher J. Mundy, Nandini Ananth *The Journal of Chemical Physics* **164**, 212501 (2026).

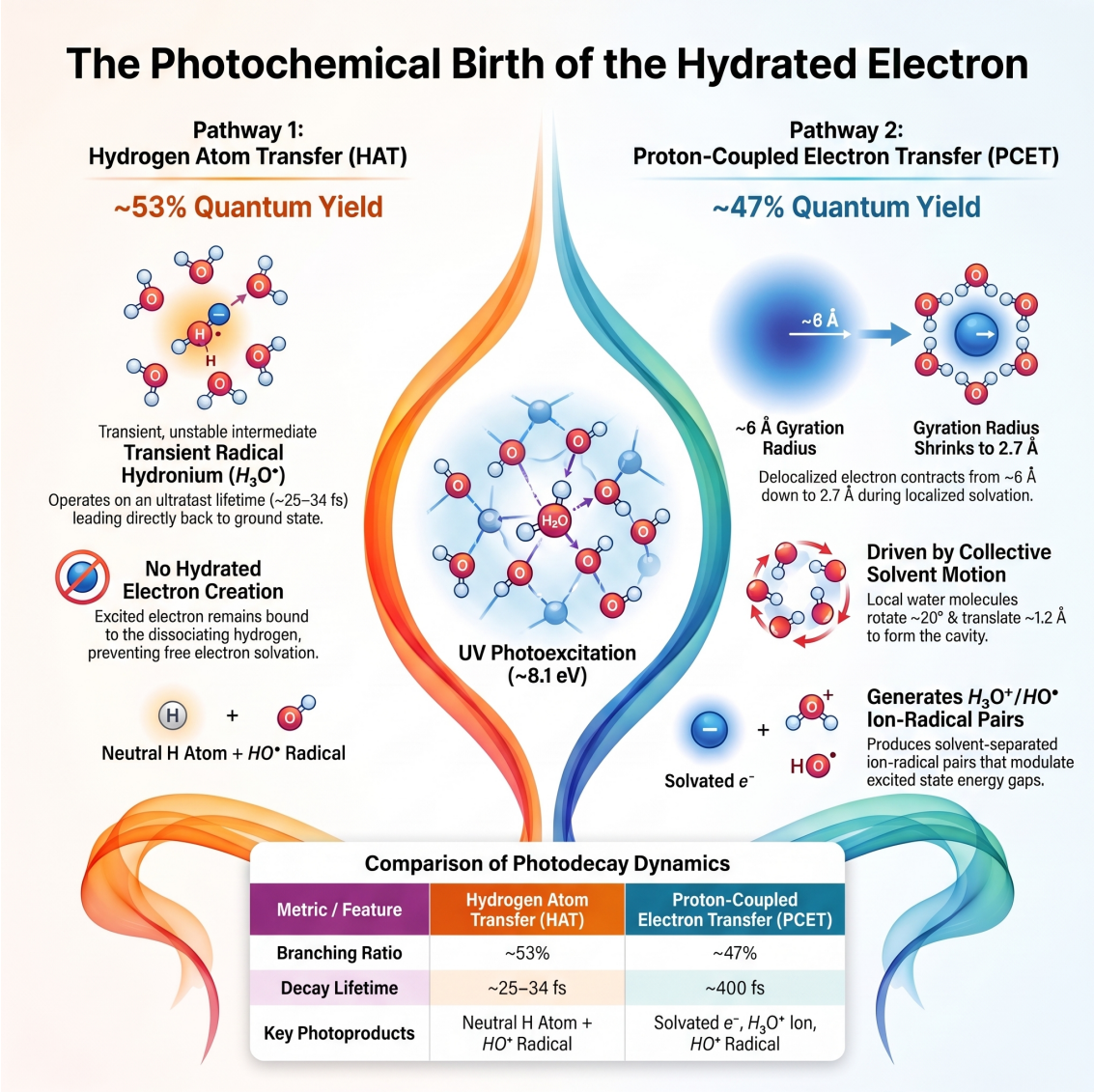
DOI: https://doi.org/10.1063/5.0327460



Lattice-scale variations in viscosity are correlated with solution structure at mineral-water interfaces

Elias Nakouzi, Haoyuan Shi, Jaeyoung Heo, James J. De Yoreo, Christopher J. Mundy, Greg A. Kimmel, Gregory K. Schenter, Jaehun Chun *Journal of Colloid and Interface Science* **718**, 140475 (2026).

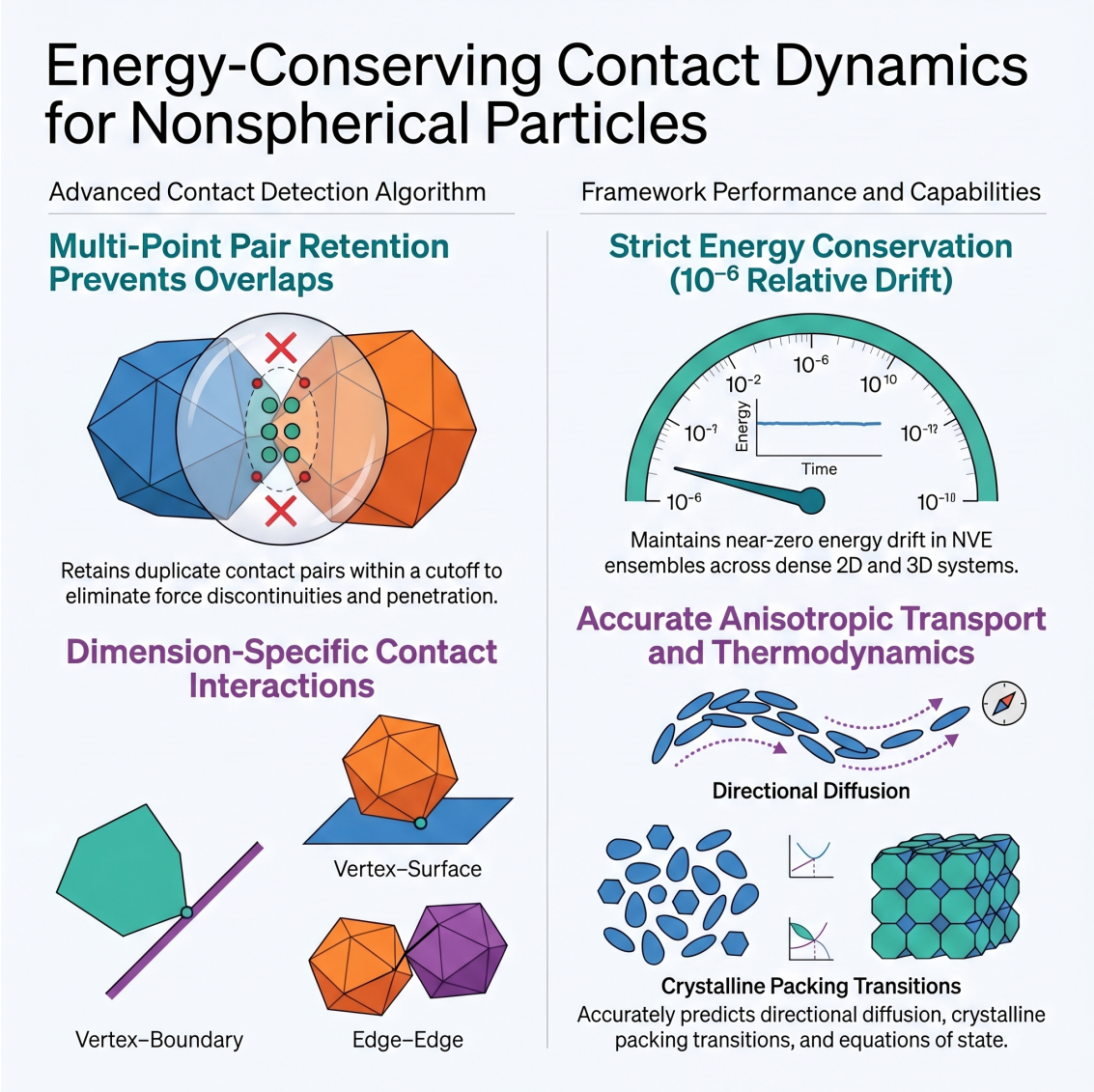
DOI: https://doi.org/10.1016/j.jcis.2026.140475



Simulating the Photochemical Birth of the Hydrated Electron in Liquid Water

Gonzalo Díaz Mirón, Cesare Malosso, Solana Di Pino, Colin K. Egan, Diganta Dasgupta, Christopher J. Mundy, Ali Hassanali *Nature Communications* **17**, 3764 (2026).

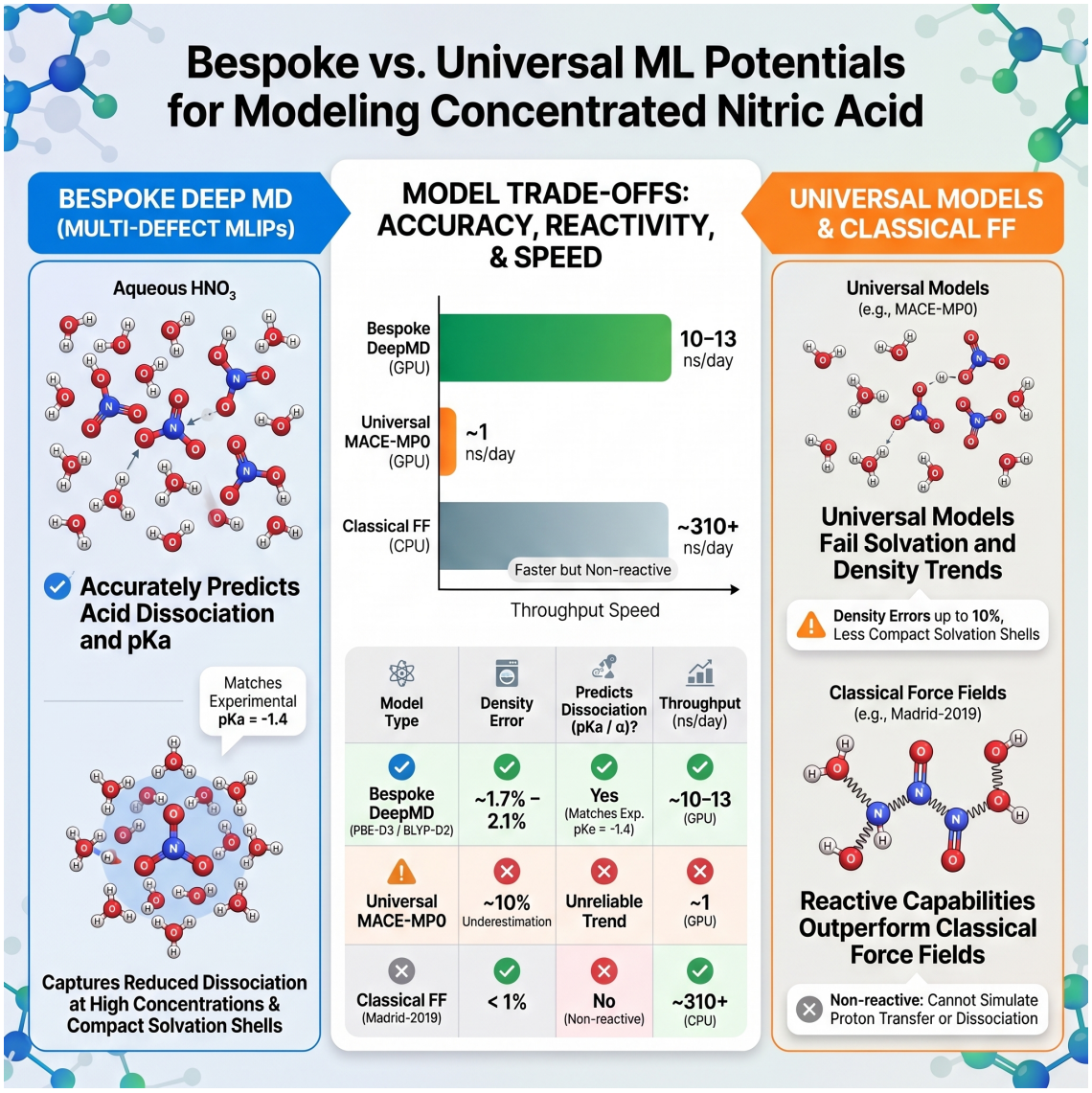
DOI: https://doi.org/10.1038/s41467-026-70045-7



Energy-conserving contact dynamics of nonspherical rigid-body particles

Haoyuan Shi, Christopher J. Mundy, Gregory K. Schenter, Jaehun Chun *APL Computational Physics* **2**, 016108 (2026).

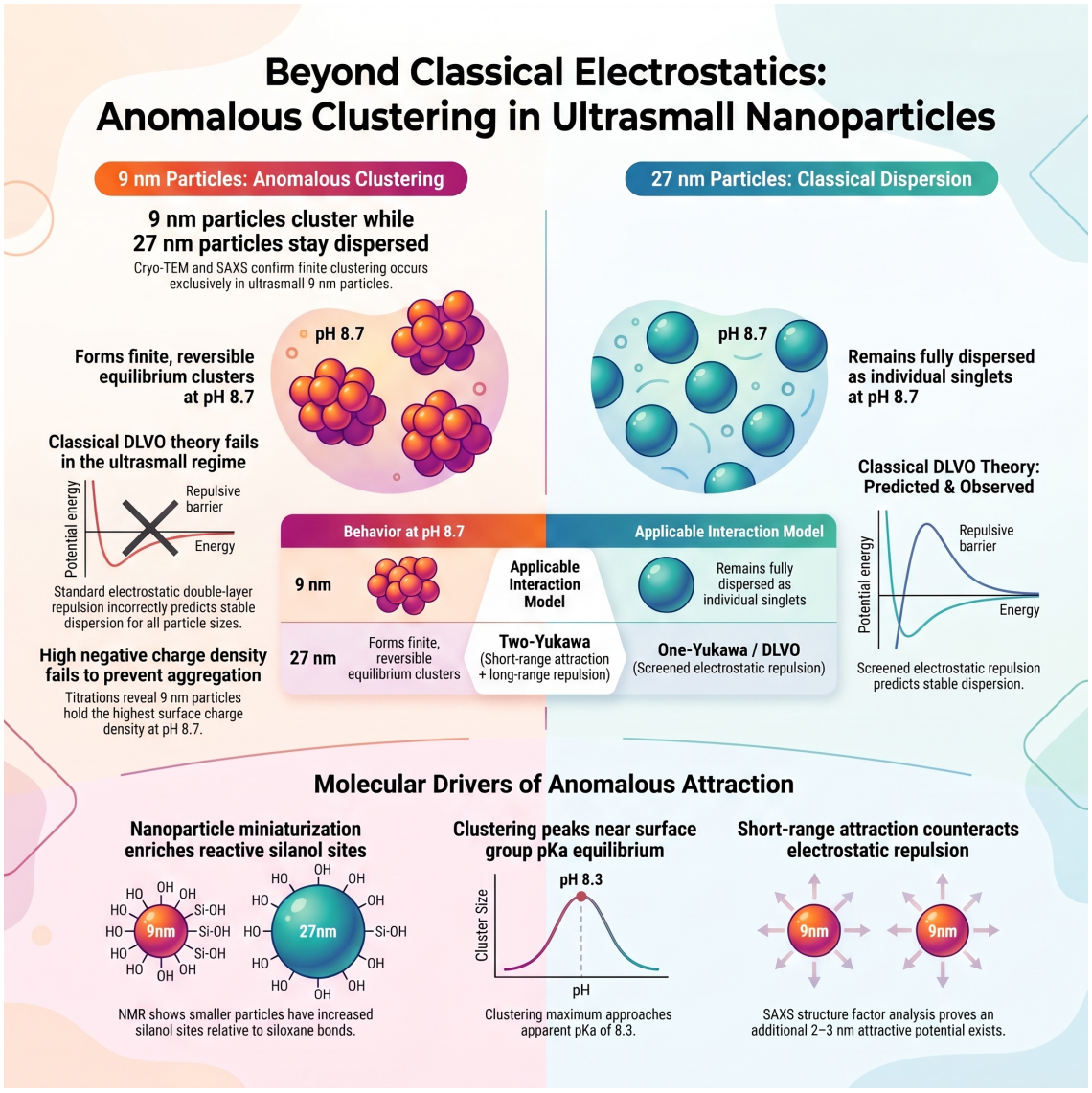
DOI: https://doi.org/10.1063/5.0319853



Modeling the behavior of concentrated aqueous HNO3 using machine learning interatomic potentials

Mohammadhasan Dinpajooh, Michael D. Lacount, Scott E. Muller, Neil J. Henson, Daniel Mejia-Rodriguez, Axel Gomez, Christopher J. Mundy, Andrew M. Ritzmann *The Journal of Chemical Physics* **164**, 014504 (2026).

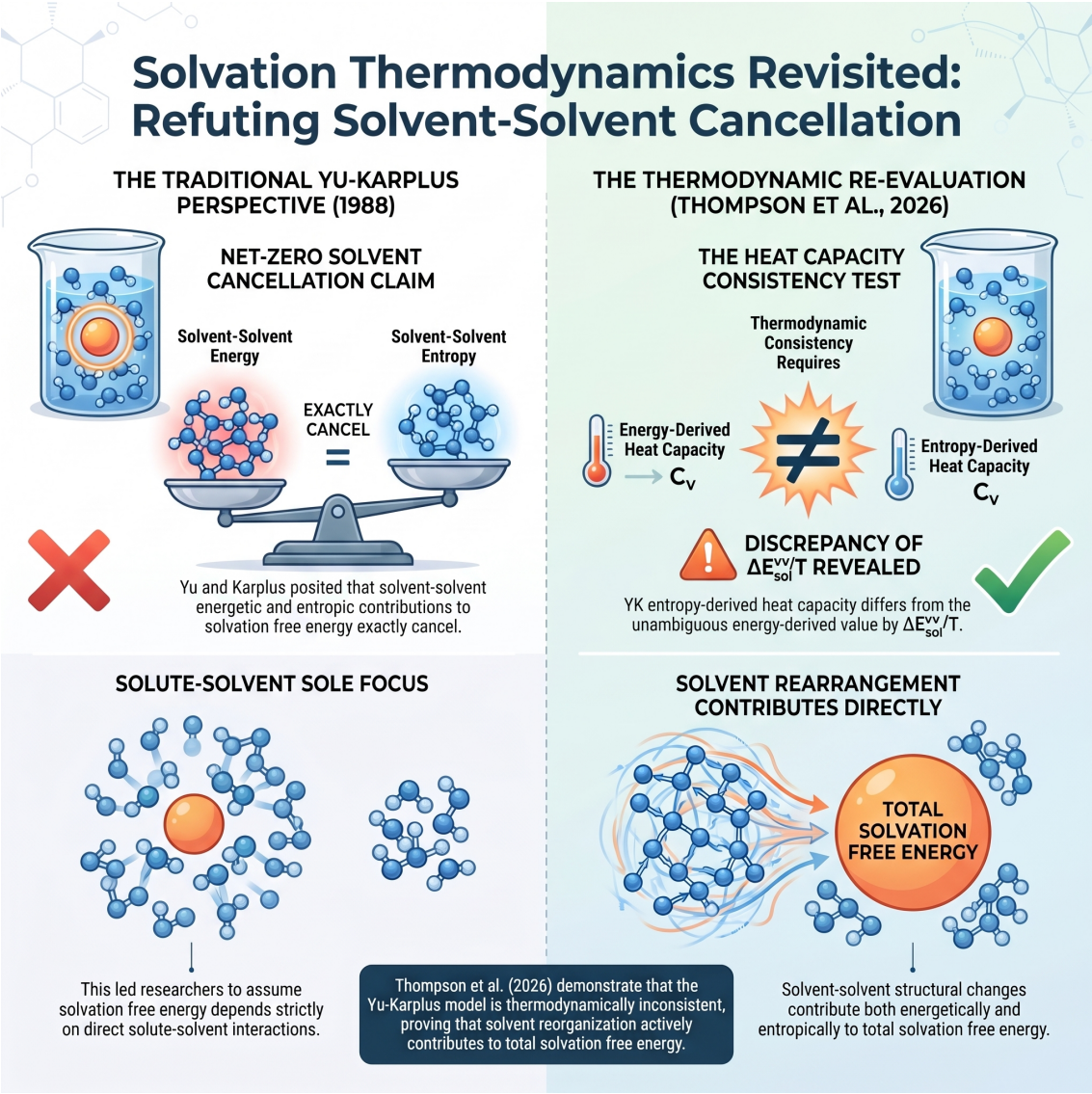
DOI: https://doi.org/10.1063/5.0303907



Molecular Surface Chemistry Drives Anomalous Clustering of Ultrasmall Silica Nanoparticles

Ruchi Patel, Gernot Rother, Noshir Pesika, Greg A. Kimmel, Yan Levin, Gregory K. Schenter, Christopher J. Mundy, Jaehun Chun, Bhuvnesh Bharti *The Journal of Physical Chemistry Letters* **17**, 8270-8276 (2026).

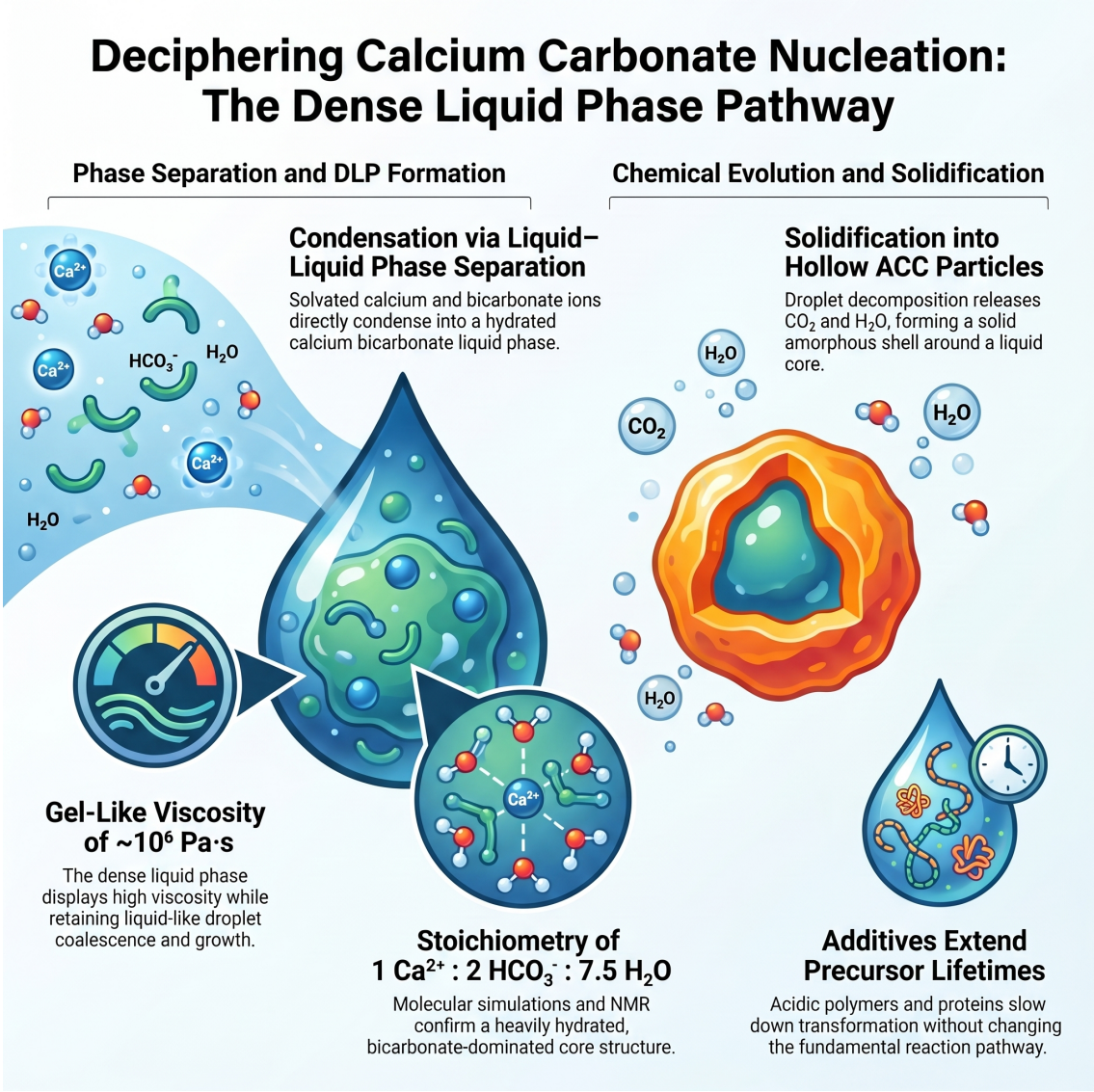
DOI: https://doi.org/10.1021/acs.jpclett.6c01796



Solvation thermodynamics revisited

Ward H. Thompson, Gregory K. Schenter, Christopher J. Mundy, Brian B. Laird *The Journal of Chemical Physics* **165**, 104108 (2026).

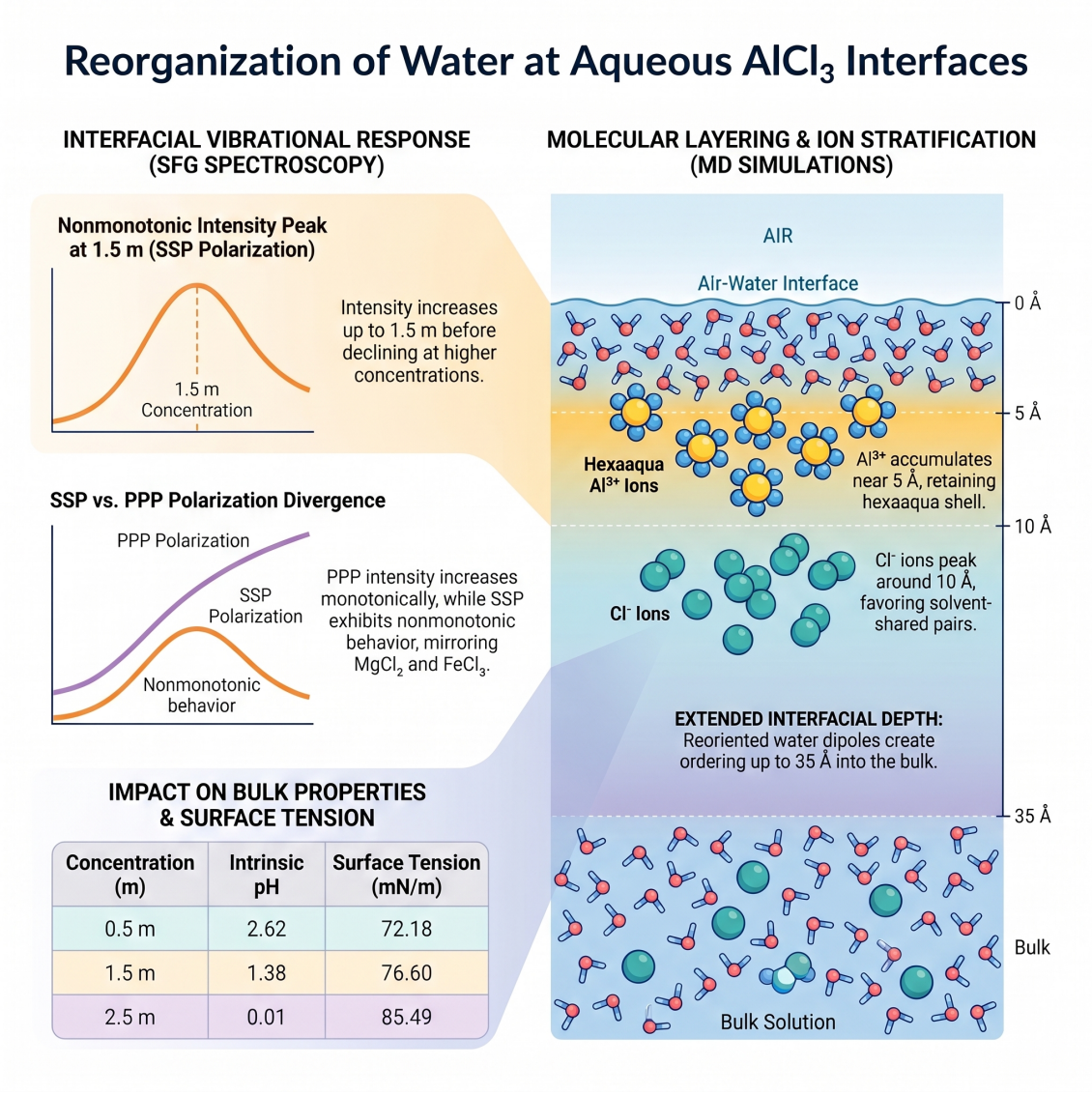
DOI: https://doi.org/10.1063/5.0346490



Formation, chemical evolution and solidification of the dense liquid phase of calcium (bi)carbonate

Biao Jin, Ying Chen, Harley Pyles, Marcel D. Baer, Benjamin A. Legg, Zheming Wang, Nancy M. Washton, Karl T. Mueller, David Baker, Gregory K. Schenter, Christopher J. Mundy, James J. De Yoreo *Nature Materials* **24**, 125-132 (2025).

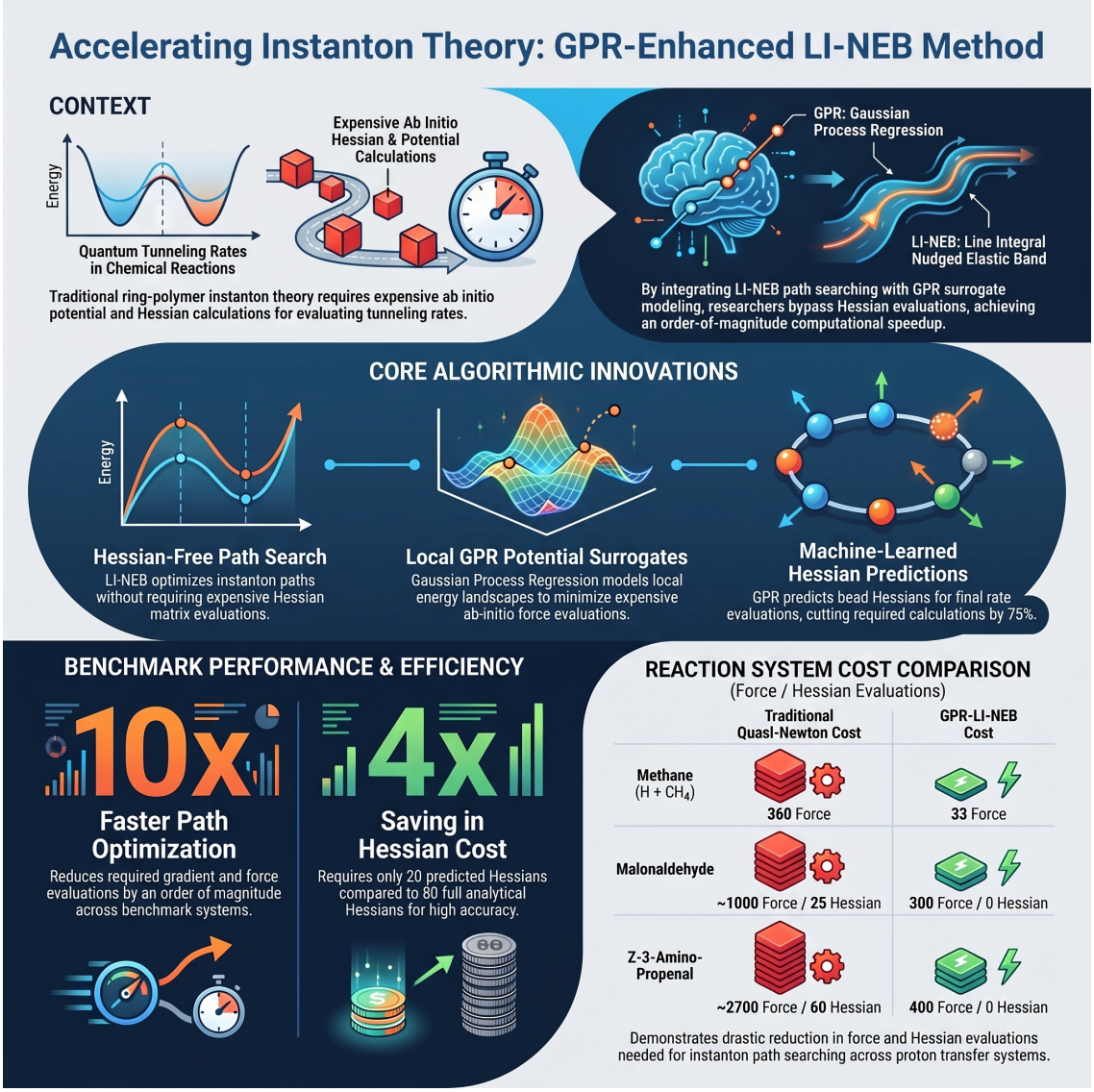
DOI: https://doi.org/10.1038/s41563-024-02025-5



Reorganization of Water at Aqueous Aluminum Chloride ($AlCl_3$) Interfaces: Vibrational Sum Frequency Generation and Molecular Dynamics Simulations

Biswajit Biswas, Mohammadhasan Dinpajooh, Gwendolyn Nieto, Narendra Adhikari, Gregory K. Schenter, Shawn M. Kathmann, Christopher J. Mundy, Heather C. Allen *The Journal of Physical Chemistry A* **129**, 10616-10631 (2025).

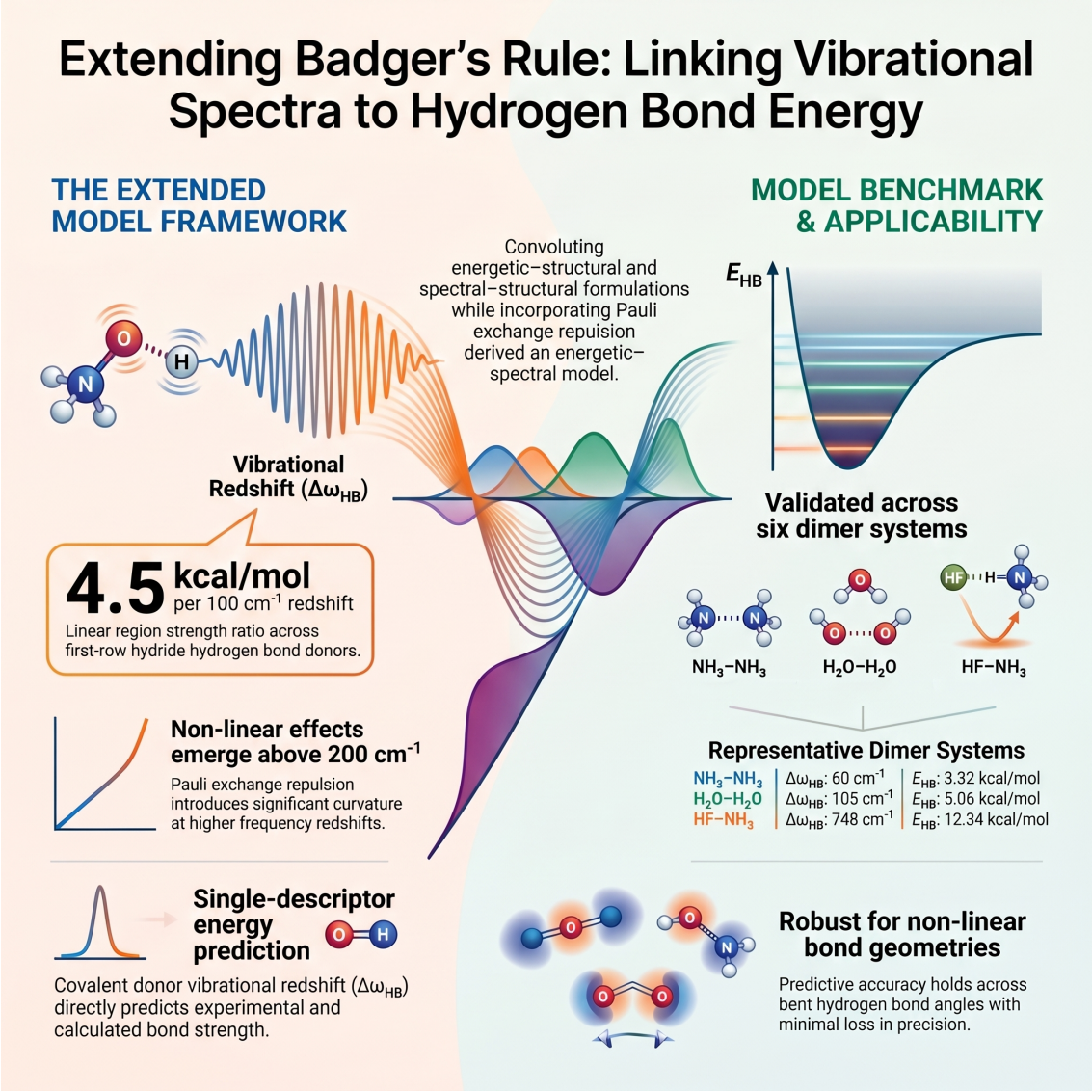
DOI: https://doi.org/10.1021/acs.jpca.5c03910



Accelerating Instanton Theory with the Line Integral Nudged Elastic Band Method and Gaussian Process Regression

Chenghao Zhang, Amke Nimmrich, Britta A. Johnson, Gregory K. Schenter, Munira Khalil, Niranjan Govind *Journal of Chemical Theory and Computation* **21**, 7517-7534 (2025).

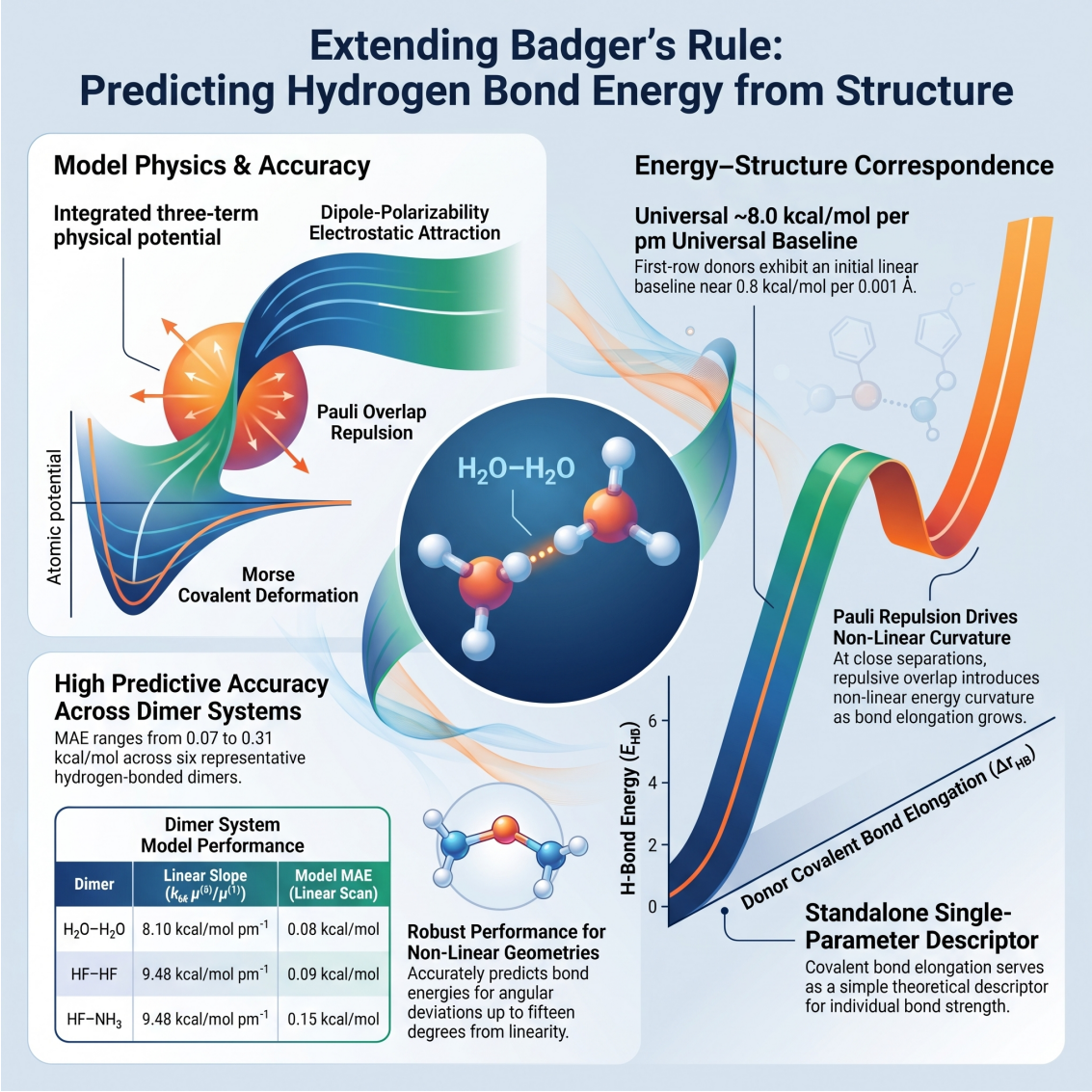
DOI: https://doi.org/10.1021/acs.jctc.5c00673



Extending Badger's rule. II. The relationship between energy and vibrational spectra in hydrogen bonds

Garrett D. Santis, Sotiris S. Xantheas *The Journal of Chemical Physics* **162**, 244121 (2025).

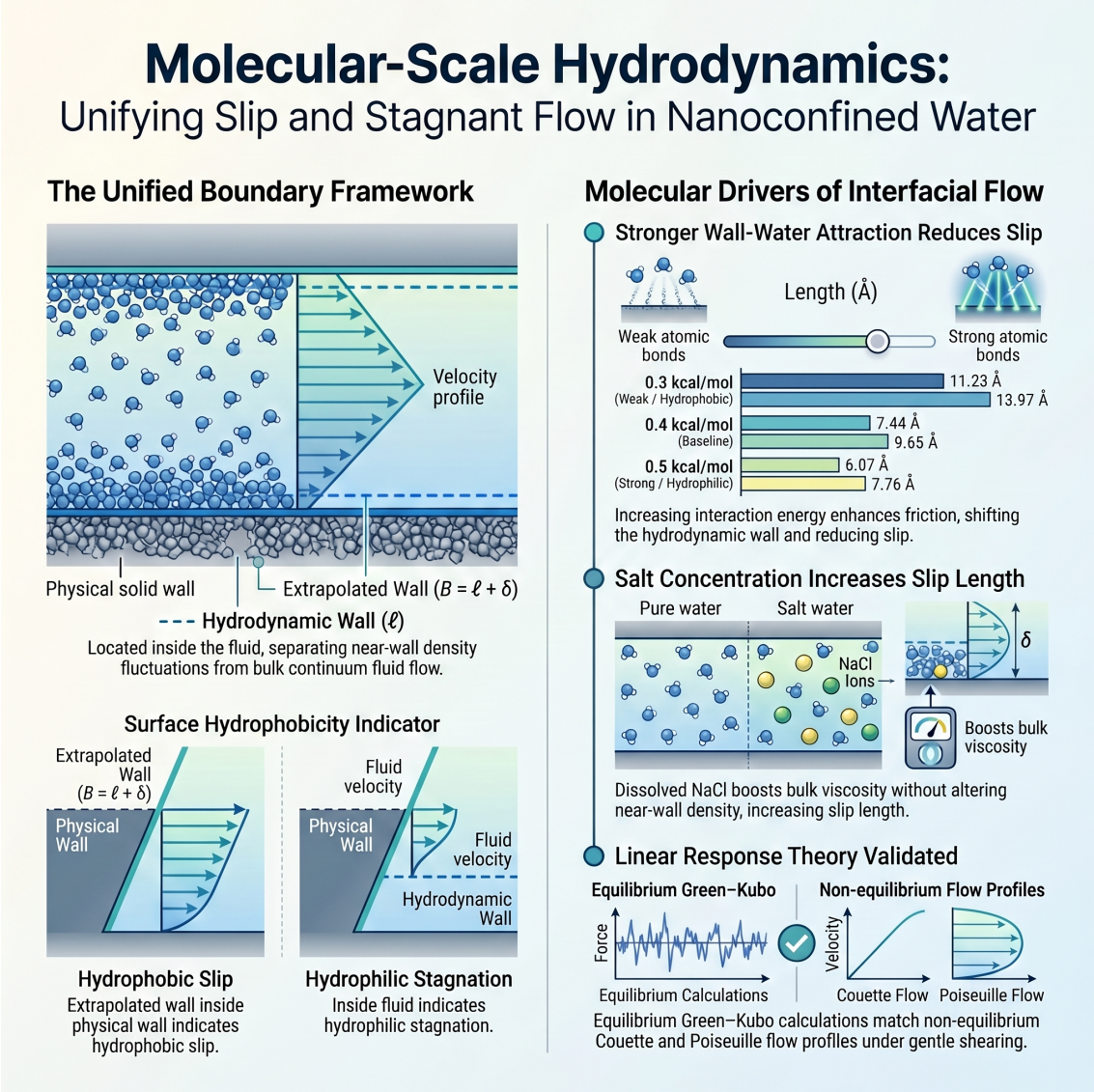
DOI: https://doi.org/10.1063/5.0263484



Extending Badger's rule. I. The relationship between energy and structure in hydrogen bonds

Garrett D. Santis, Sotiris S. Xantheas *The Journal of Chemical Physics* **162**, 044106 (2025).

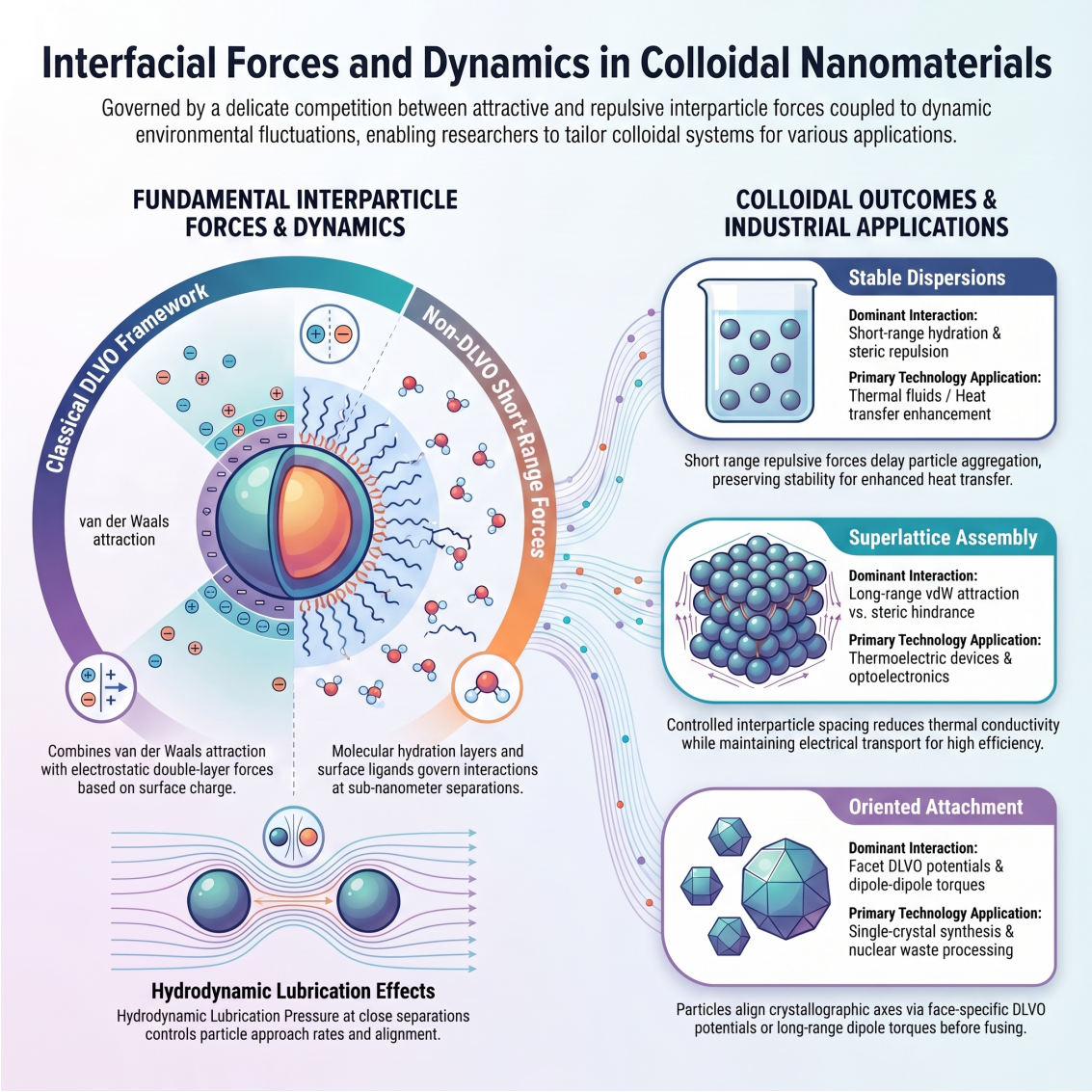
DOI: https://doi.org/10.1063/5.0244238



Incorporating the molecular-scale into a hydrodynamic description of confined aqueous systems

Haoyuan Shi, Christopher J. Mundy, Gregory K. Schenter, Jaehun Chun *The Journal of Chemical Physics* **163**, 134708 (2025).

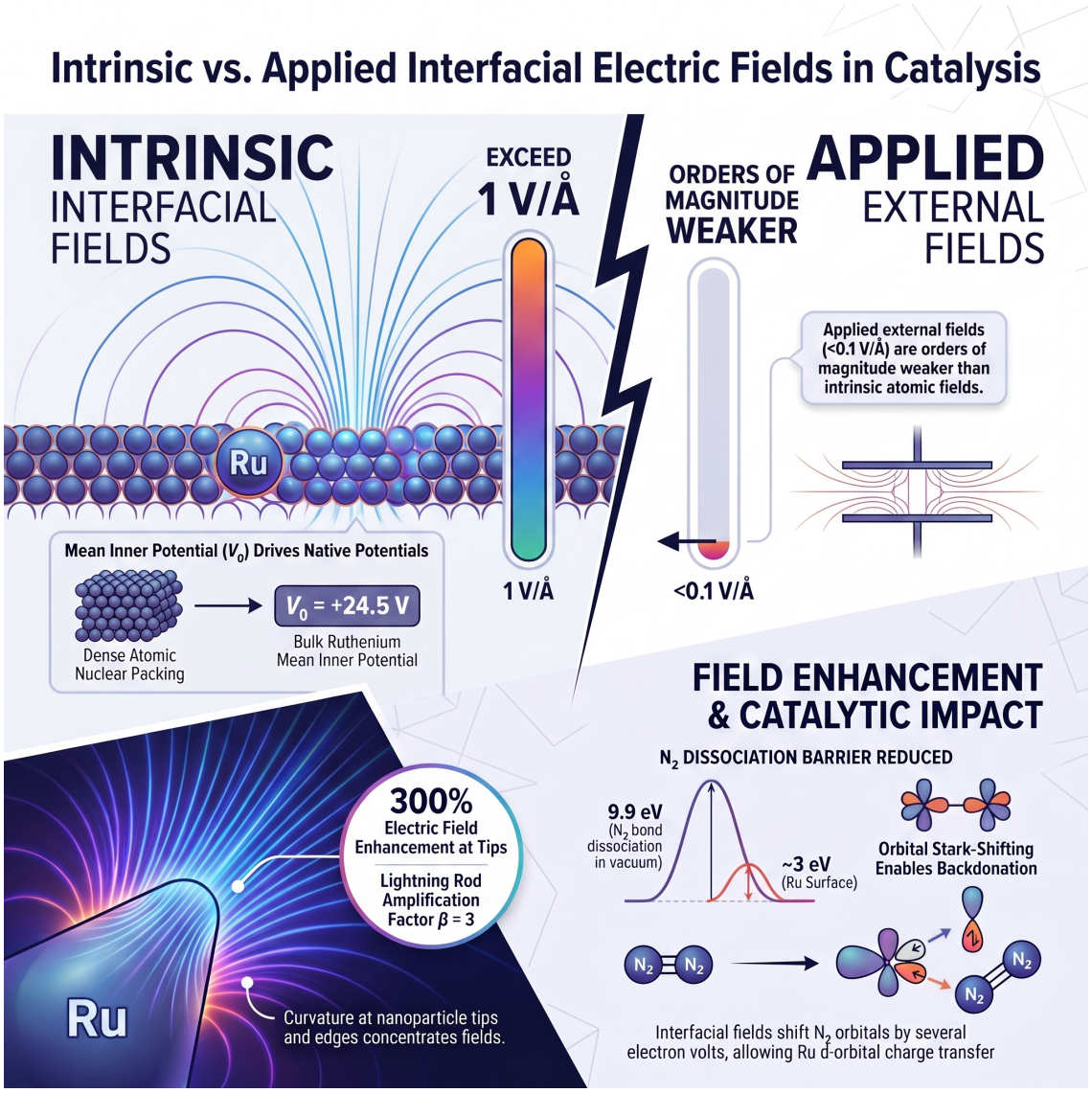
DOI: https://doi.org/10.1063/5.0279626



Colloidal phenomena reflect the interplay between interfacial solution structure, interparticle forces, and dynamical response

Jaeyoung Heo, Pravalika Butreddy, Gregory K. Schenter, Christopher J. Mundy, James J. De Yoreo, Elias Nakouzi, Jaewon Lee, Jaehun Chun *Current Opinion in Colloid & Interface Science* **75**, 101887 (2025).

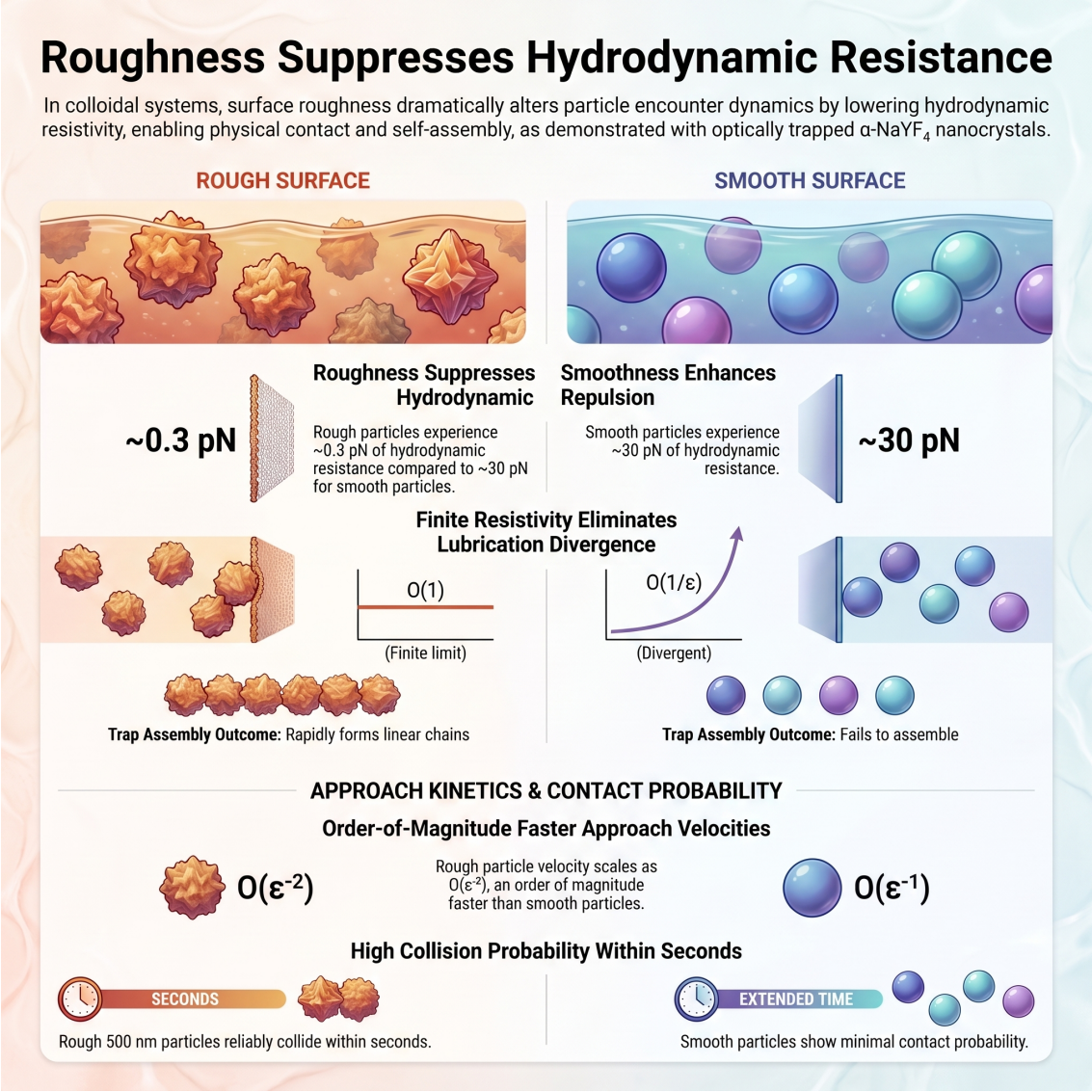
DOI: https://doi.org/10.1016/j.cocis.2024.101887



Electric Fields at Interfaces

Michael D. LaCount, Sten V. Lambeets, Daniel E. Perea, Tanya Prozorov, Shawn M. Kathmann *The Journal of Physical Chemistry C* **129**, 15489-15506 (2025).

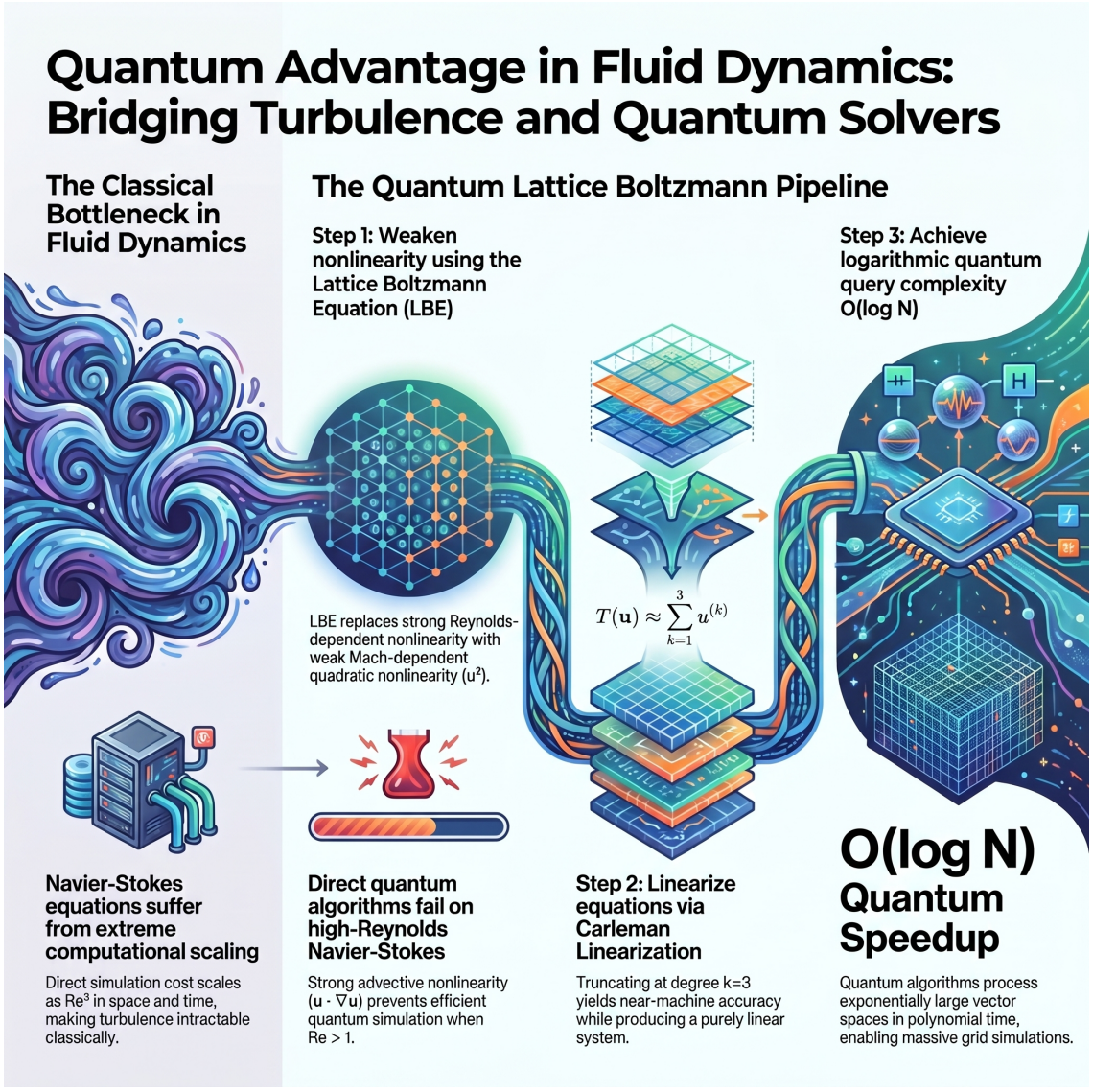
DOI: https://doi.org/10.1021/acs.jpcc.5c04104



Mediation of Colloidal Encounter Dynamics by Surface Roughness

Robert G. Felsted, Jaehun Chun, Gregory K. Schenter, Alexander B. Bard, Xiaojing Xia, Peter J. Pauzauskie *Physical Review Letters* **134**, 088201 (2025).

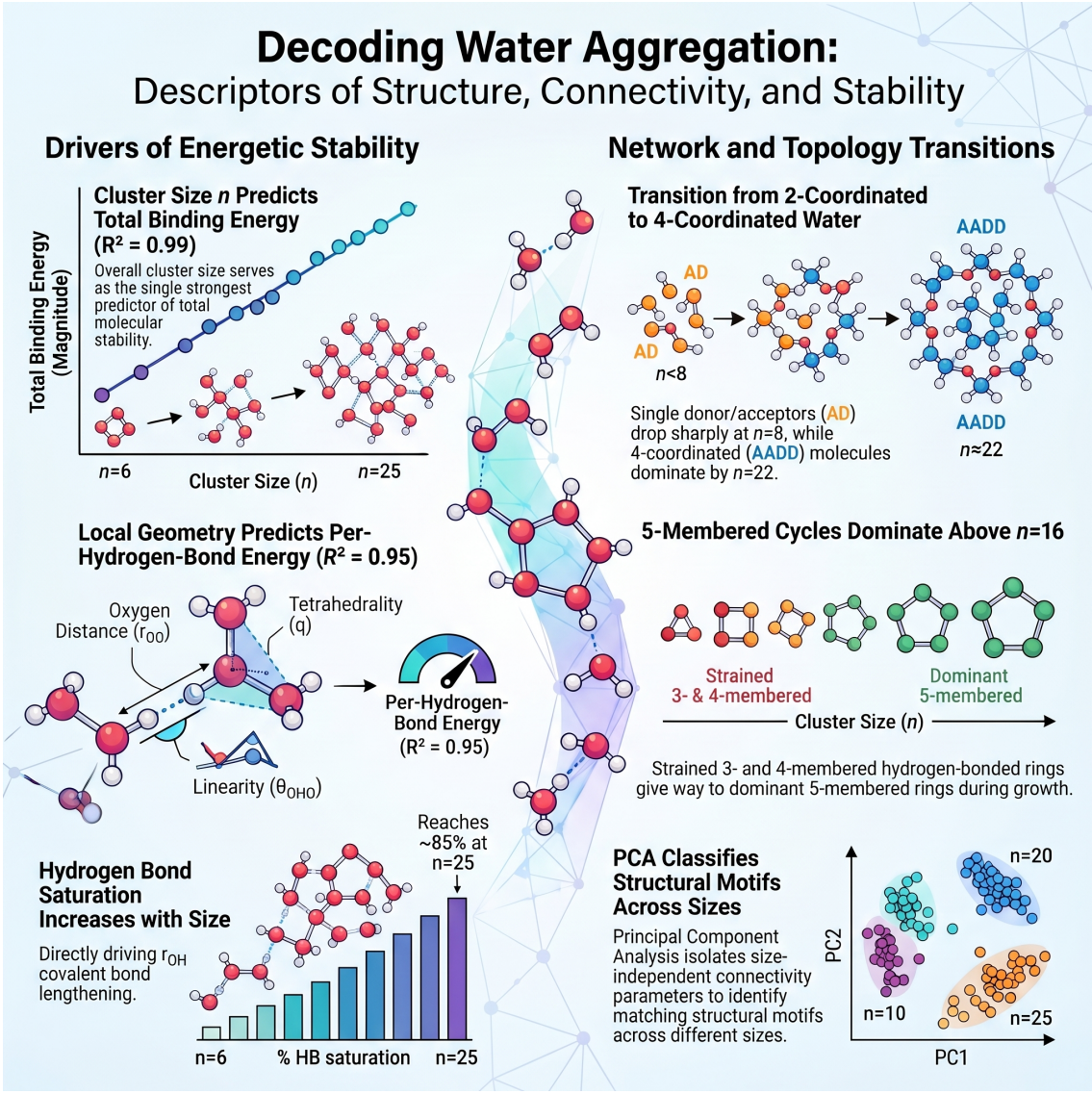
DOI: https://doi.org/10.1103/physrevlett.134.088201



Potential quantum advantage for simulation of fluid dynamics

Xiangyu Li, Xiaolong Yin, Nathan Wiebe, Jaehun Chun, Gregory K. Schenter, Margaret S. Cheung, Johannes Mülmenstädt *Physical Review Research* **7**, 013036 (2025).

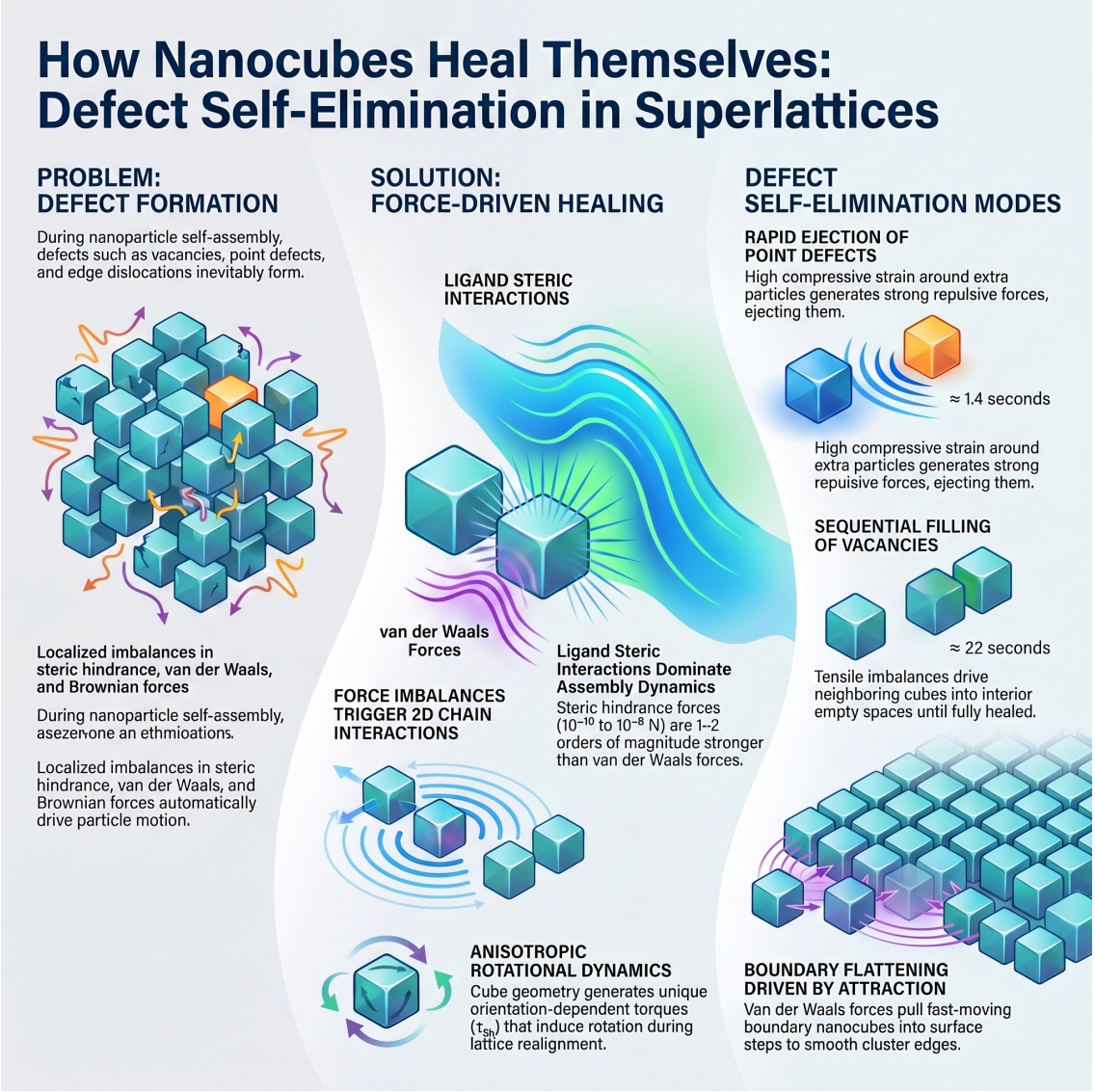
DOI: https://doi.org/10.1103/physrevresearch.7.013036



Descriptors of water aggregation

Garrett D. Santis, Kristina M. Herman, Joseph P. Heindel, Sotiris S. Xantheas *The Journal of Chemical Physics* **160**, 054306 (2024).

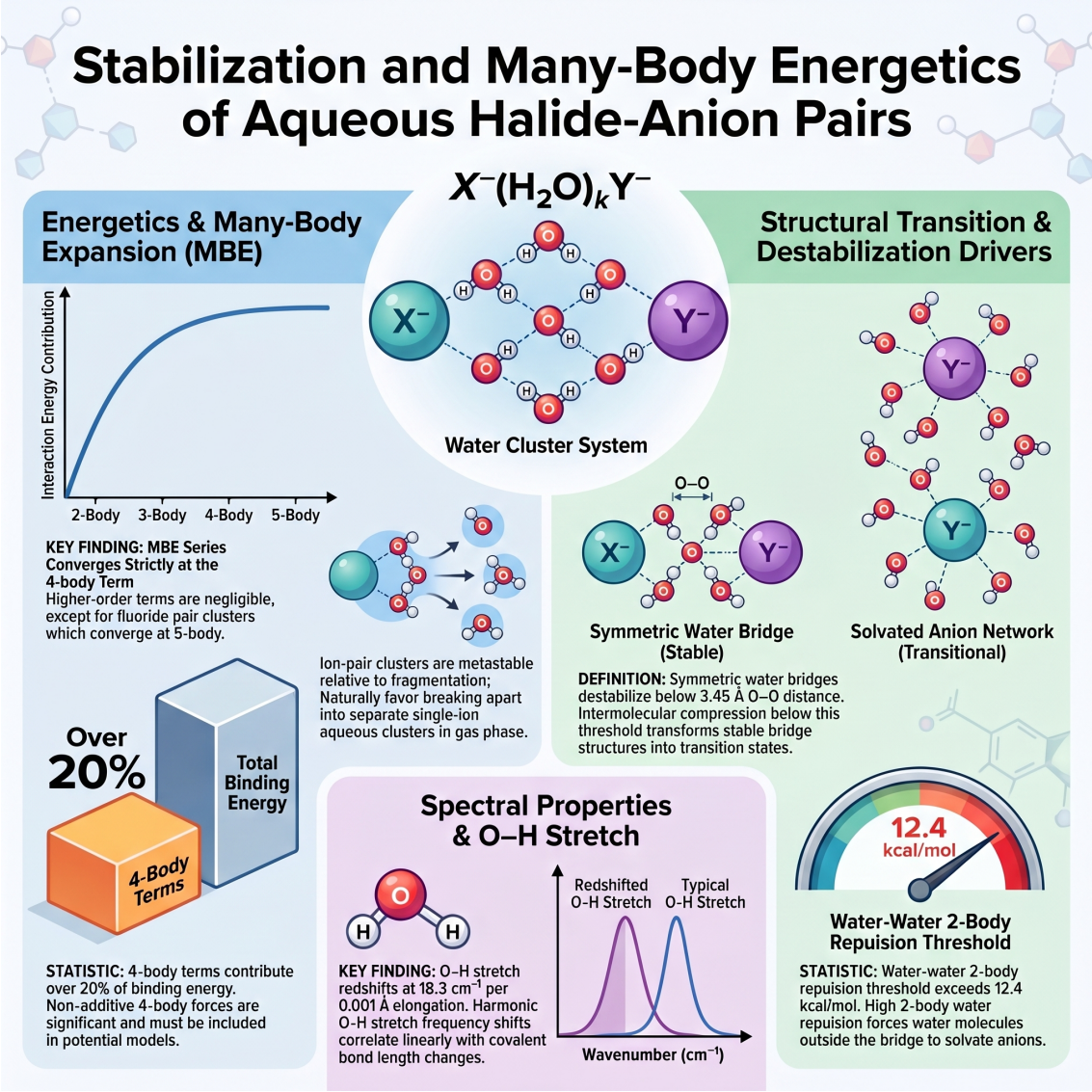
DOI: https://doi.org/10.1063/5.0179815



Defect Self-Elimination in Nanocube Superlattices Through the Interplay of Brownian, van der Waals, and Ligand-Based Forces and Torques

Jaewon Lee, Zexi Lu, Zhigang Wu, Colin Ophus, Gregory K. Schenter, James J. De Yoreo, Jaehun Chun, Dongsheng Li *ACS Nano* **18**, 32386-32400 (2024).

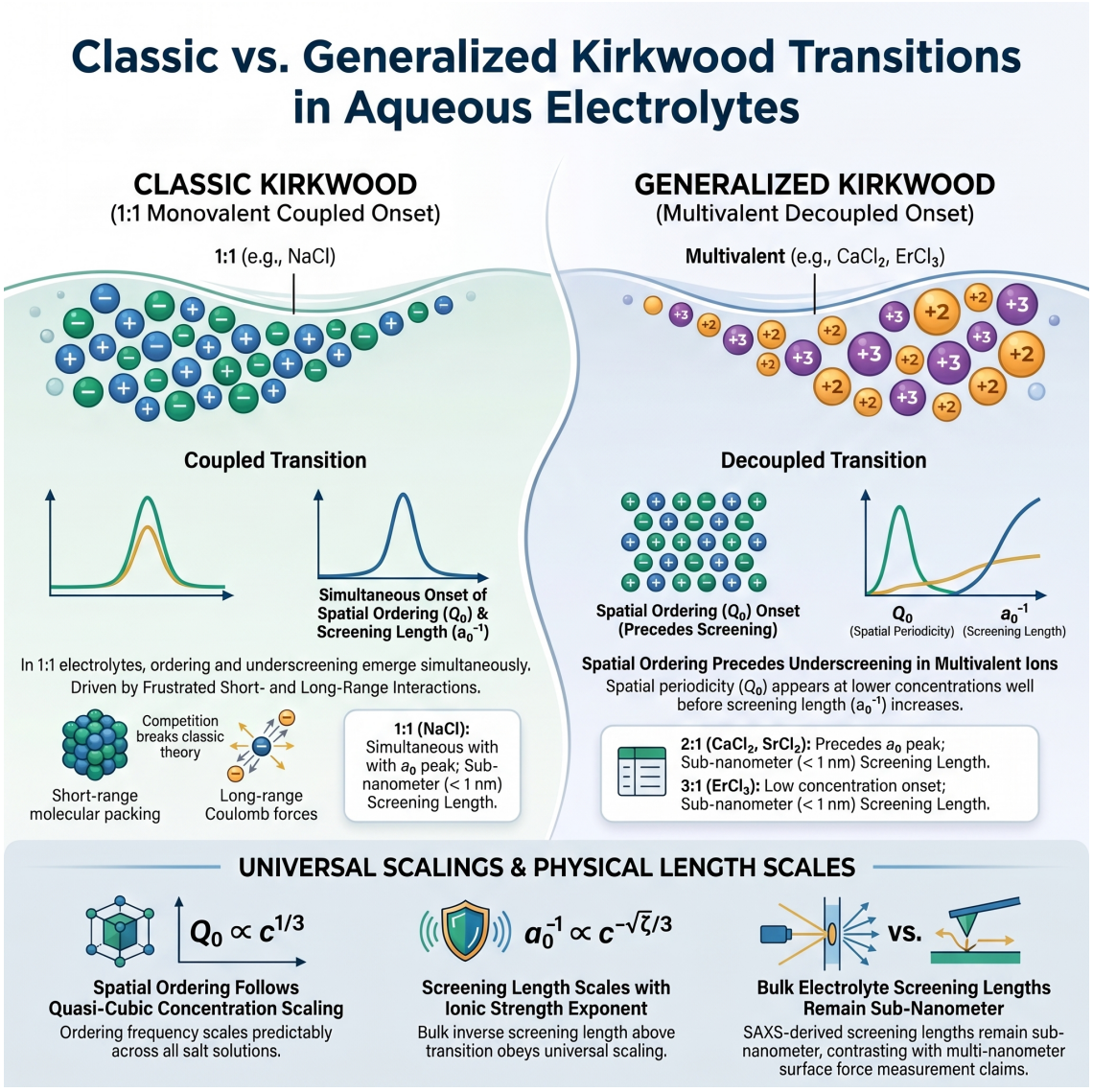
DOI: https://doi.org/10.1021/acsnano.3c08610



The Many-Body Expansion for Aqueous Systems Revisited: IV. Stabilization of Halide–Anion Pairs in Small Water Clusters

Maxwell P. Hoffman, Sotiris S. Xantheas *The Journal of Physical Chemistry A* **128**, 9876-9892 (2024).

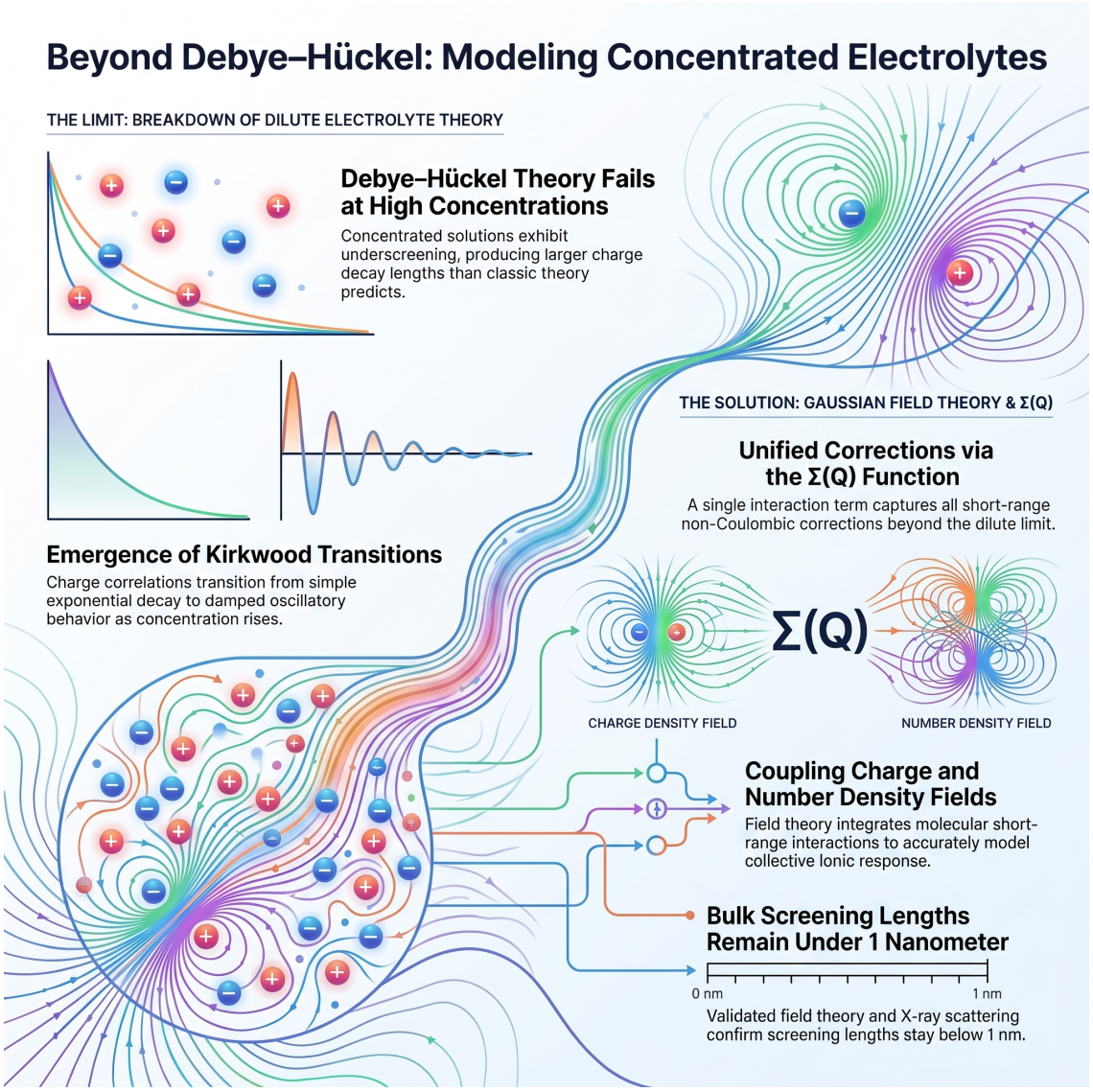
DOI: https://doi.org/10.1021/acs.jpca.4c05427



Detecting underscreening and generalized Kirkwood transitions in aqueous electrolytes

Mohammadhasan Dinpajooh, Elisa Biasin, Emily T. Nienhuis, Sebastian T. Mergelsberg, Chris J. Benmore, Gregory K. Schenter, John L. Fulton, Shawn M. Kathmann, Christopher J. Mundy *The Journal of Chemical Physics* **161**, 151102 (2024).

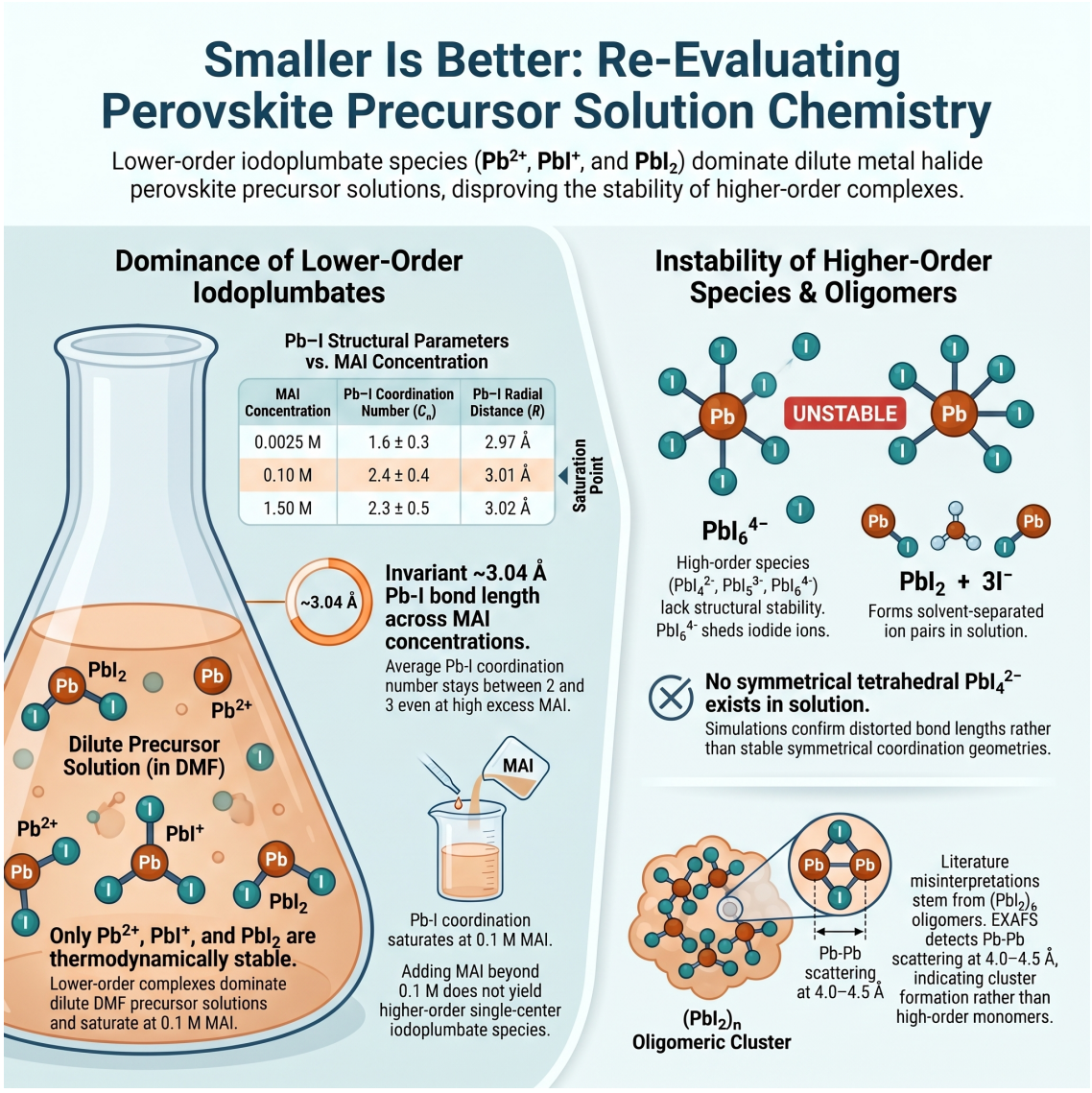
DOI: https://doi.org/10.1063/5.0234518



Beyond the Debye–Hückel limit: Toward a general theory for concentrated electrolytes

Mohammadhasan Dinpajooh, Nadia N. Intan, Timothy T. Duignan, Elisa Biasin, John L. Fulton, Shawn M. Kathmann, Gregory K. Schenter, Christopher J. Mundy *The Journal of Chemical Physics* **161**, 230901 (2024).

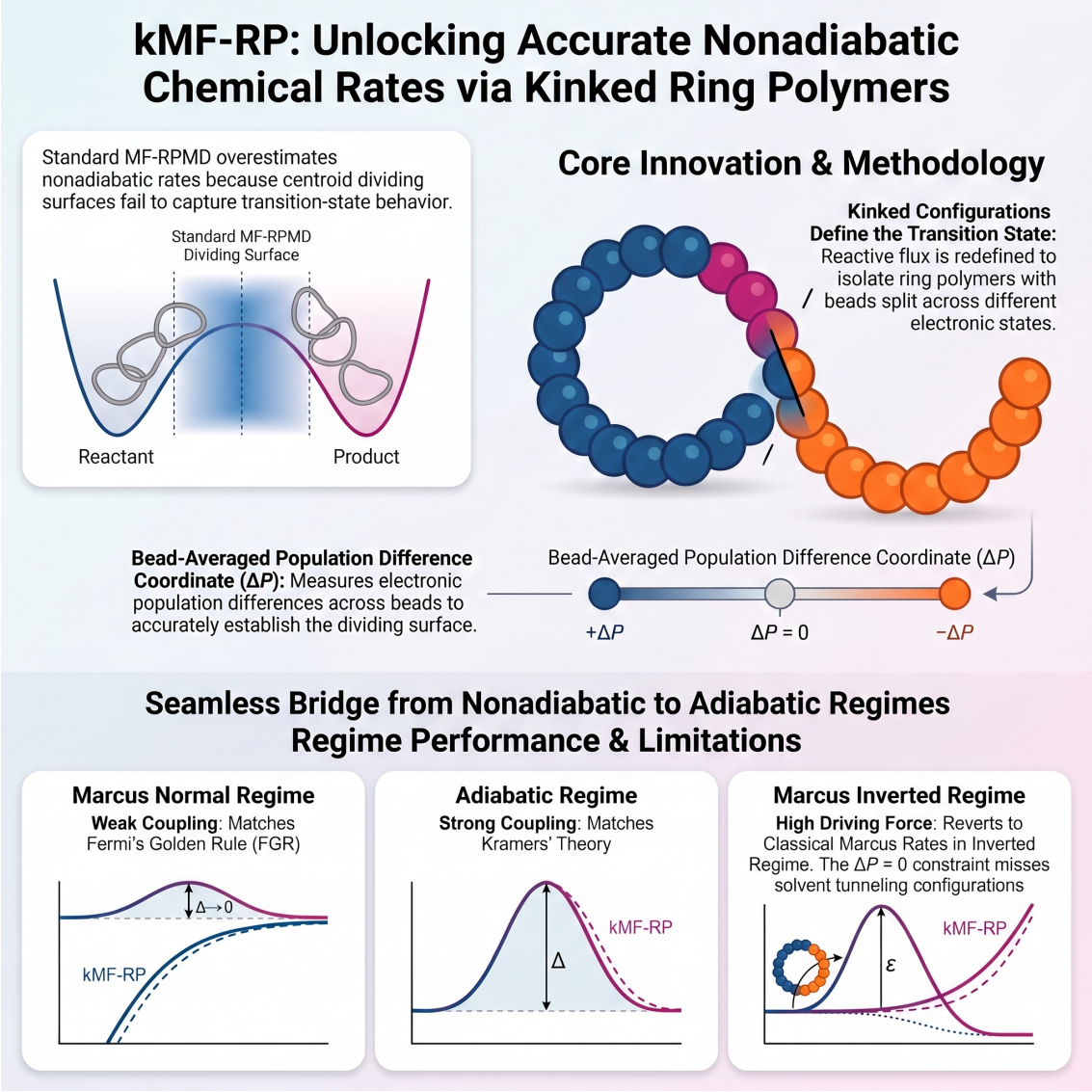
DOI: https://doi.org/10.1063/5.0238708



Smaller Is Better: The Case for Lower-Order Iodoplumbate Species Dominating $MAPbI_3$/Dimethylformamide Solutions

Nadia N. Intan, Blaire A. Sorenson, Yong Kyu Choi, Joshua J. Choi, John L. Fulton, Niranjan Govind, Shelly D. Kelly, Gregory K. Schenter, Paulette Clancy, Christopher J. Mundy *Chemistry of Materials* **36**, 8424-8436 (2024).

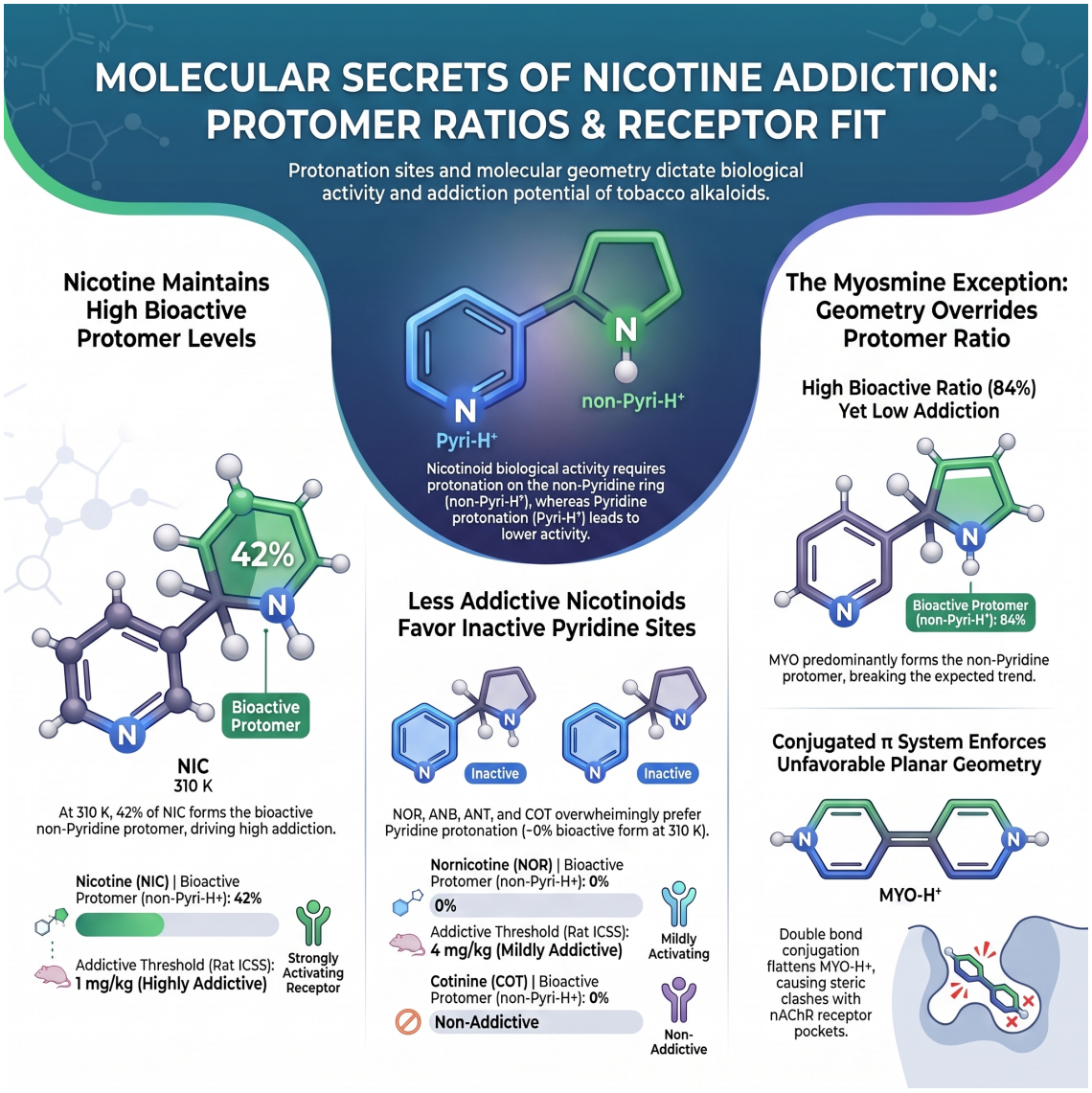
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Mean-Field Ring Polymer Rates Using a Population Dividing Surface

Nathan London, Siyu Bu, Britta Johnson, Nandini Ananth *The Journal of Physical Chemistry A* **128**, 5730-5739 (2024).

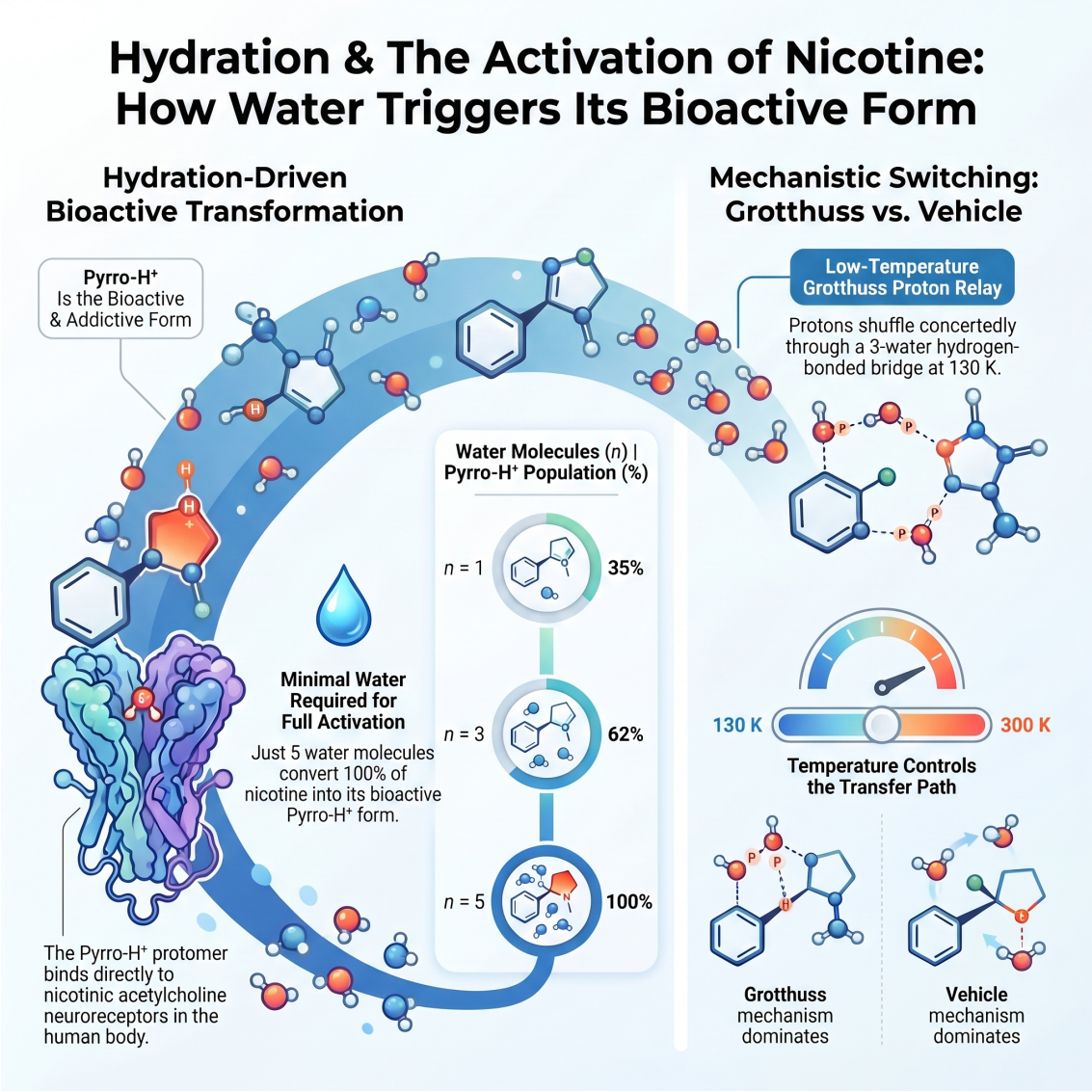
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The Gas Phase Protonation Sites of Six Naturally Occurring Nicotinoids

Yuika Okura, Garrett D. Santis, Keisuke Hirata, Sotiris S. Xantheas, Masaaki Fujii, Shun-Ichi Ishiuchi *The Journal of Physical Chemistry Letters* **15**, 6966-6973 (2024).

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Switching of Protonation Sites in Hydrated Nicotine via a Grotthuss Mechanism

Yuika Okura, Garrett D. Santis, Keisuke Hirata, Vasilios S. Melissas, Shun-ichi Ishiuchi, Masaaki Fujii, Sotiris S. Xantheas *Journal of the American Chemical Society* **146**, 3023-3030 (2024).

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