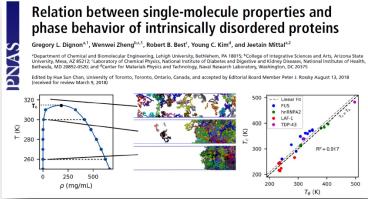
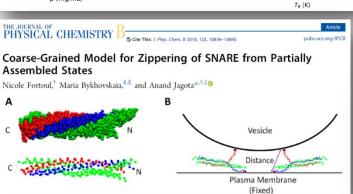
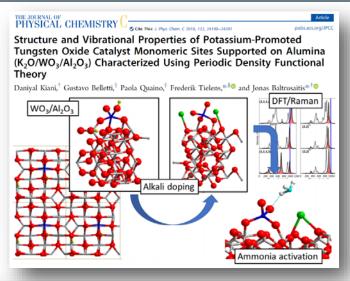
Molecular Modeling and Simulation

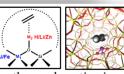






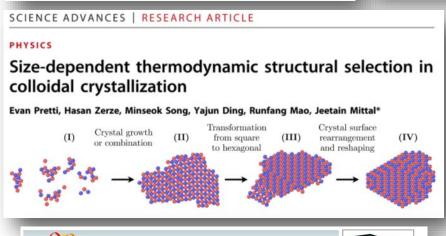




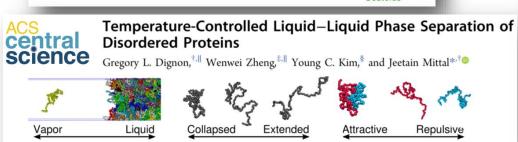


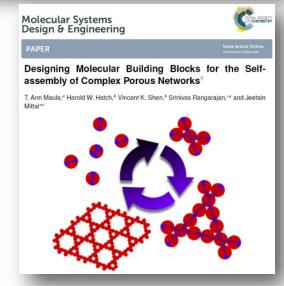
Influence of brønsted-acid and cation-exchange sites on ethene adsorption in ZSM-5

Yu-Hao Yeh^a, Christopher Rzepa^b, Srinivas Rangarajan^b, Raymond J. Gorte^{a,}*

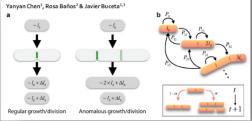












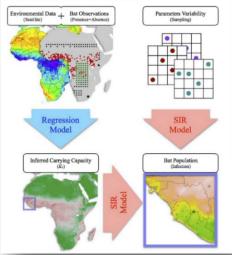
Data Science, Systems, and **Controls**

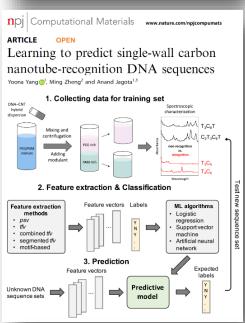




A Predictive Spatial Distribution Framework for Filovirus-Infected Bats

Graziano Fiorillo¹, Paolo Bocchini⁰ & Javier Buceta^{2,3}





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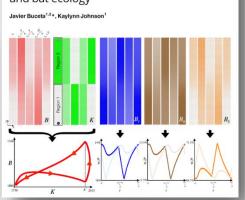
PAPER

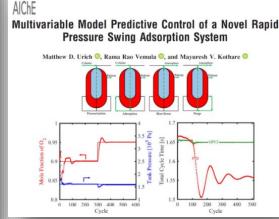
Designing compact training sets for data-driven molecular property prediction through optimal exploitation and exploration

Bowen Li and Srinivas Rangarajan*





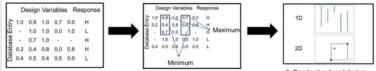






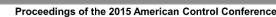
Solving Materials' Small Data Problem with Dynamic Experimental Databases

Michael McBride, Nils Persson, Elsa Reichmanis and Martha A. Grover * 0



 Develop database using published literature results and identify critical response value Sort responses according to critical value and determine maximum and minimum design variable values





Designing Closed-loop Brain-Machine Interfaces with Network of Spiking Neurons Using MPC Strategy

Hongguang Pan, Baocang Ding, Weimin Zhong, Gautam Kumar and Mayuresh V. Kothare*

