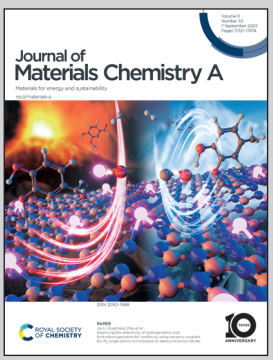
Showcasing research from Profs. Peng Bai and Subhransu Maji's laboratories, Colleges of Engineering and of Information and Computer Sciences, University of Massachusetts Amherst, Massachusetts, United States.

ZeoNet: 3D convolutional neural networks for predicting adsorption in nanoporous zeolites

A deep learning framework, ZeoNet, was developed that can rapidly and accurately predict the separation performance of zeolite materials for large, flexible molecules. ZeoNet borrows ideas from the computer vision community by viewing materials as 3-dimensional images. On a standard GPU, ZeoNet can process more than eight structures per second, compared to hours per structure using state-of-art computer simulations, with an accuracy of 9.3 kJ mol^{-1} in adsorption free energy for n-octadecane.

As featured in:



See Subhransu Maji, Peng Bai *et al.*, *J. Mater. Chem. A*, 2023, **11**, 17570.

ROYAL SOCIETY OF CHEMISTRY

rsc.li/materials-a

Registered charity number: 207890