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Materials Highlight - Machine learned interatomic potential for high-throughput phonon calculations of metal-organic frameworks

Speaker Alin-Marin Elena

Join via Zoom: https://ukri.zoom.us/j/92256378528

Metal-organic frameworks (MOFs) are promising materials for applications like carbon capture, but predicting their phonon-mediated properties (e.g., thermal expansion, mechanical stability) is difficult using traditional DFT due to their complex structures. Existing machine learning models, such as MACE-MP-0, accurately predict MOF structures but fall short on phonon properties.

We have developed MACE-MP-MOF0, a fine-tuned machine learning model, and a new workflow to address this. Trained on a diverse dataset of 127 MOFs, MACE-MP-MOF0 significantly improves phonon density of states accuracy and corrects imaginary phonon modes, enabling precise, high-throughput phonon calculations. The model successfully predicts thermal expansion and bulk moduli consistent with DFT and experimental data, demonstrating its potential for guiding MOF design in energy storage and thermoelectrics.