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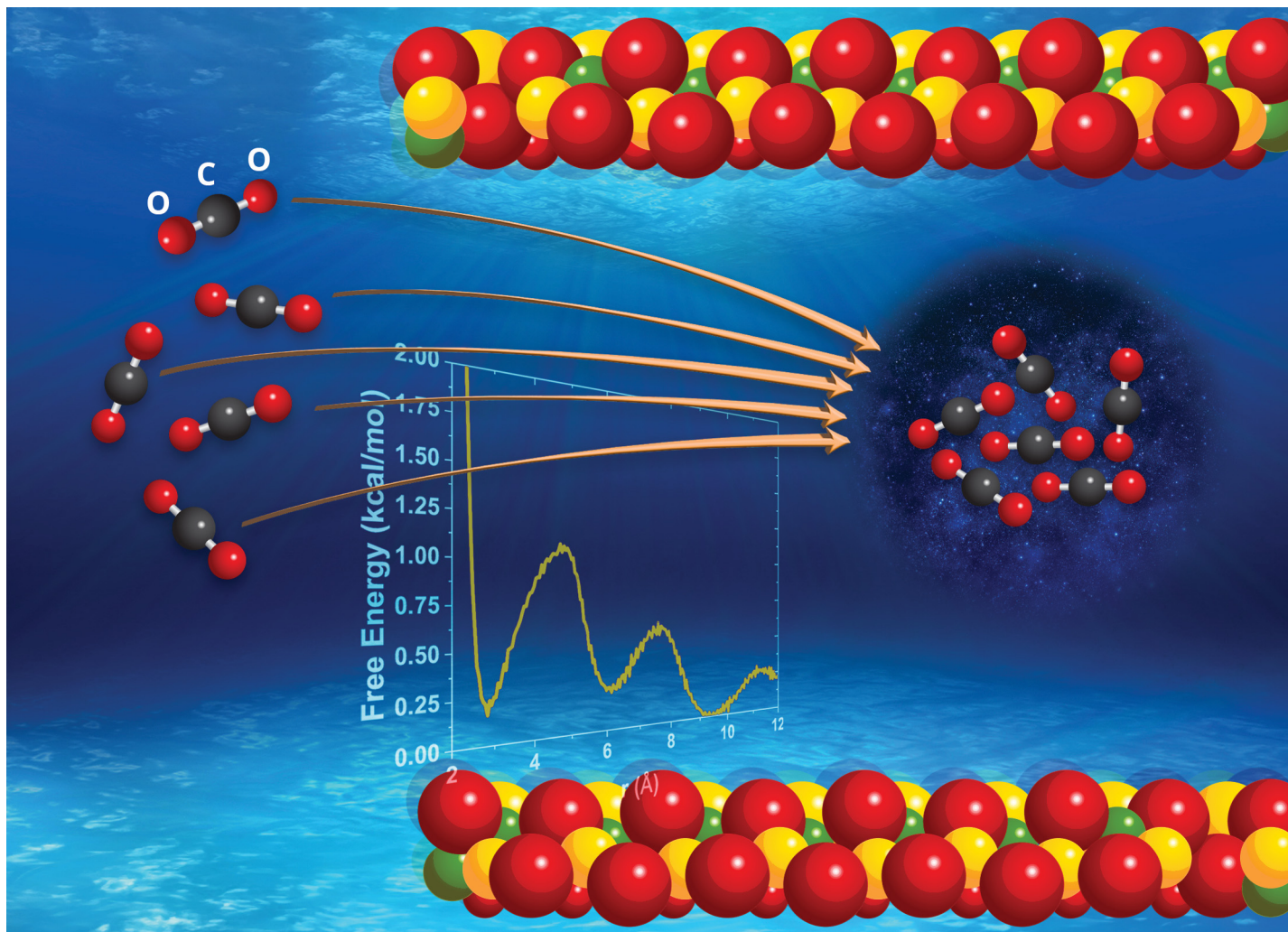


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Showcasing research from the group of Dr Tuan Ho at the Geochemistry Department, Sandia National Laboratories, NM, USA.

Confinement-induced clustering of H₂ and CO₂ gas molecules in hydrated nanopores

This computational study unveils the clustering mechanism of H₂ and CO₂ gases within hydrated nanopores, leveraging advanced free energy calculations. Our findings underscore the profound influence of nanoconfinement, surface hydrophobicity, and gas molecule chemistry on clustering. Enhanced formation of gas dimer and cluster in hydrated nanopores increases the amount of gas accumulating in the nanopores, which affects many applications including geological storage and carbon capture and sequestration.

As featured in:



See Aditya Choudhary and Tuan A. Ho, *Phys. Chem. Chem. Phys.*, 2024, **26**, 10506.