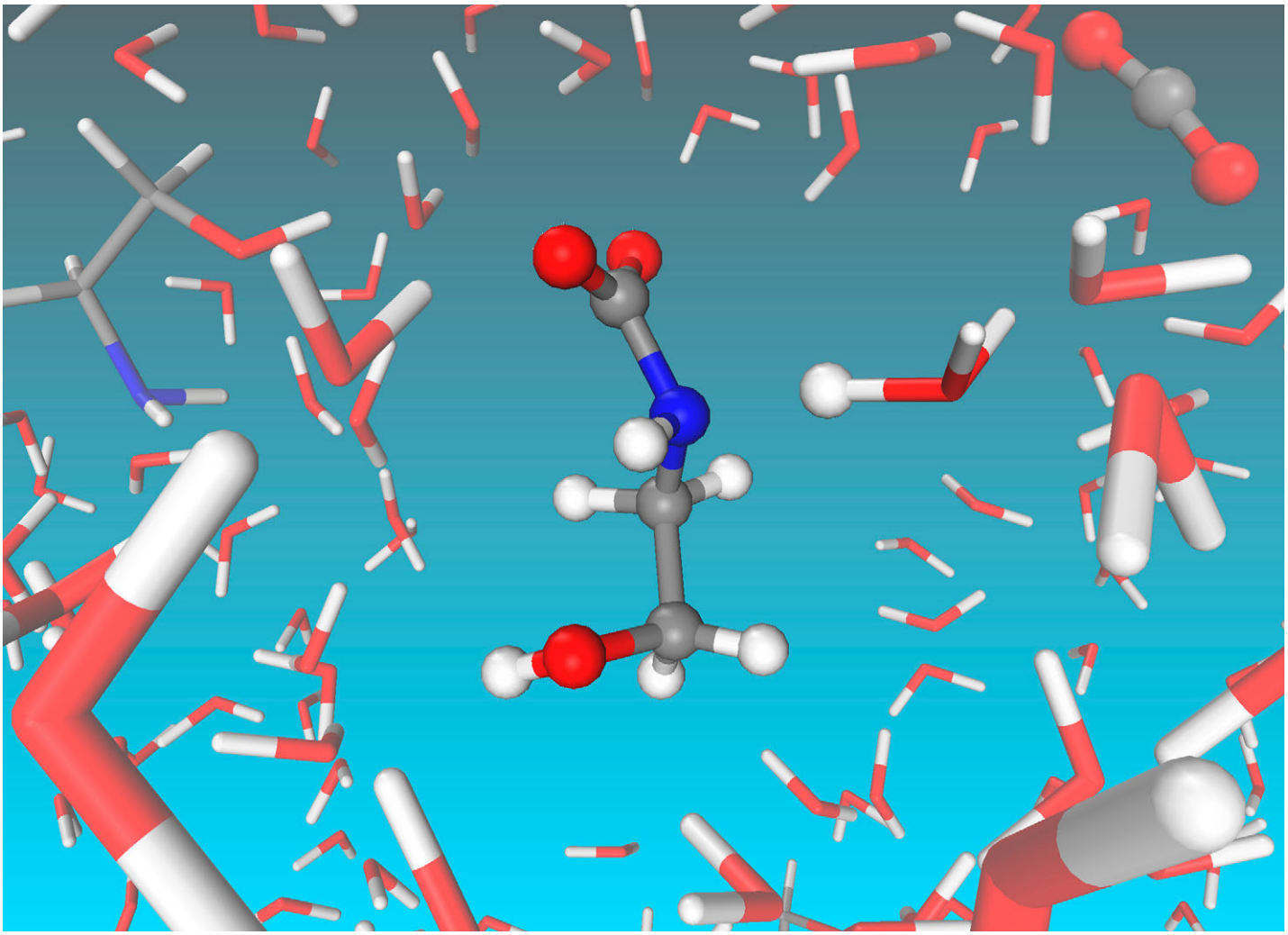

Showcasing research from the laboratory of Professor Gyeong S. Hwang at the University of Texas at Austin.

Title: Reaction mechanisms of aqueous monoethanolamine with carbon dioxide: a combined quantum chemical and molecular dynamics study

Molecular mechanisms underlying the reaction of aqueous MEA with CO_2 are examined using *ab initio* and classical molecular dynamics simulations combined with static quantum chemical calculations, with special attention to the influence of solvent structure and dynamics. This work highlights the critical role of H_2O molecules, particularly their availability and arrangement around zwitterionic intermediates, in the progression of competing CO_2 capture and solvent regeneration processes. This improved understanding can contribute to developing more comprehensive kinetic models for use in modeling and optimizing the CO_2 capture process.

As featured in:

See Gyeong S. Hwang *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 831.

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