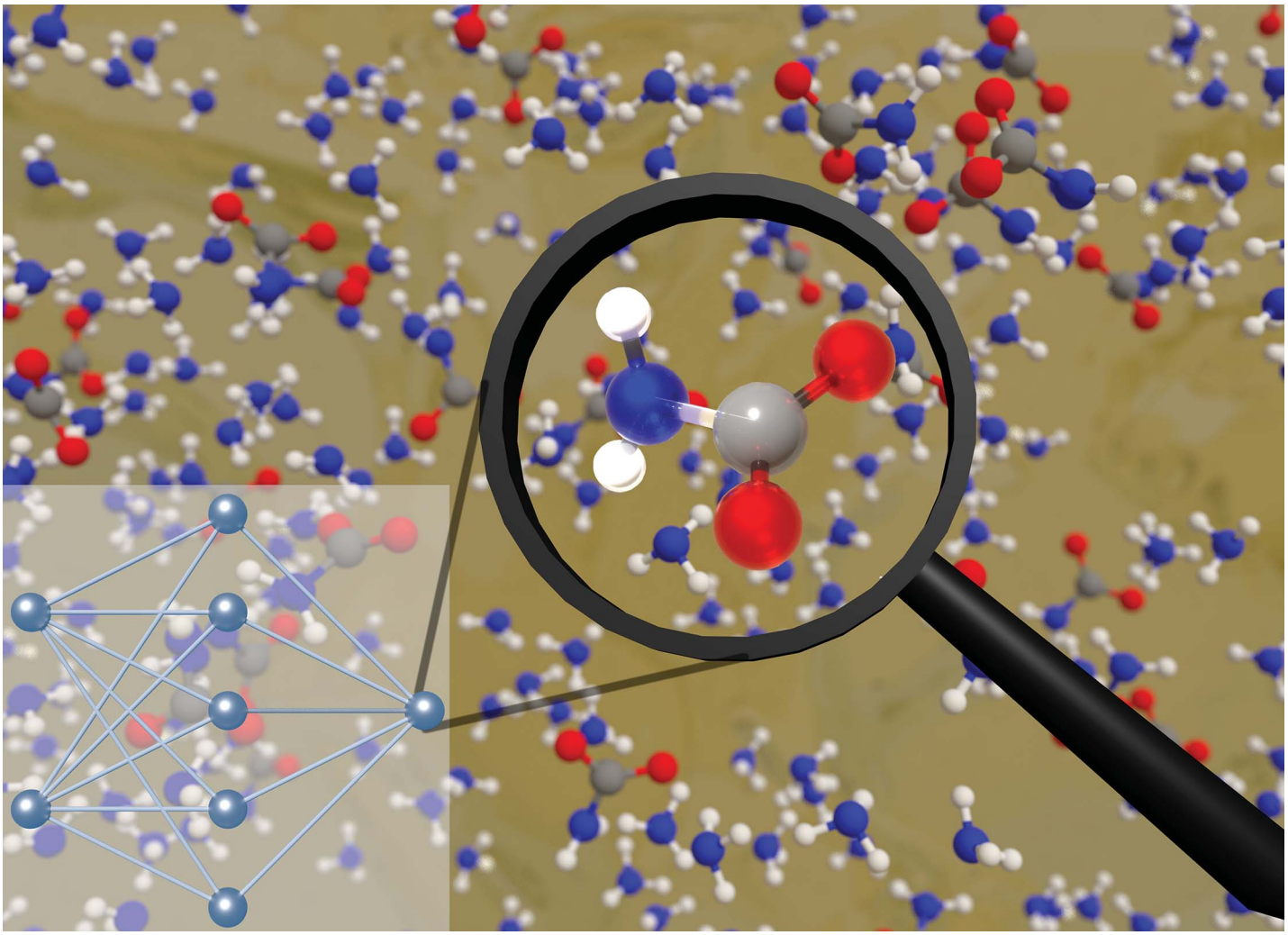

Showcasing research from Dr. Pang's group, Materials Science Division, Lawrence Livermore National Laboratory, California, USA.

Machine learning demonstrates the impact of proton transfer and solvent dynamics on CO_2 capture in liquid ammonia

Computer simulations aided by machine learning unveiled the chemical mechanism of CO_2 chemisorption in liquid ammonia. The simulations highlight the key role of solvent-mediated proton transfer to form the most stable CO_2-bound species in condensed phase. In addition, the products of this reaction (carbamate and carbamic acid) impose a significant slowdown in solvent translational and rotational dynamics. The methodology proposed in this work can be extended to amines with more complex chemical structures, paving way to the computational design of more efficient sorbents for the direct air capture of CO_2.

Artist credit: Liam Krauss / LLNL.

As featured in:

See Marcos F. Calegari Andrade, Sichi Li, Simon H. Pang *et al.*, *Chem. Sci.*, 2024, **15**, 13173.

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