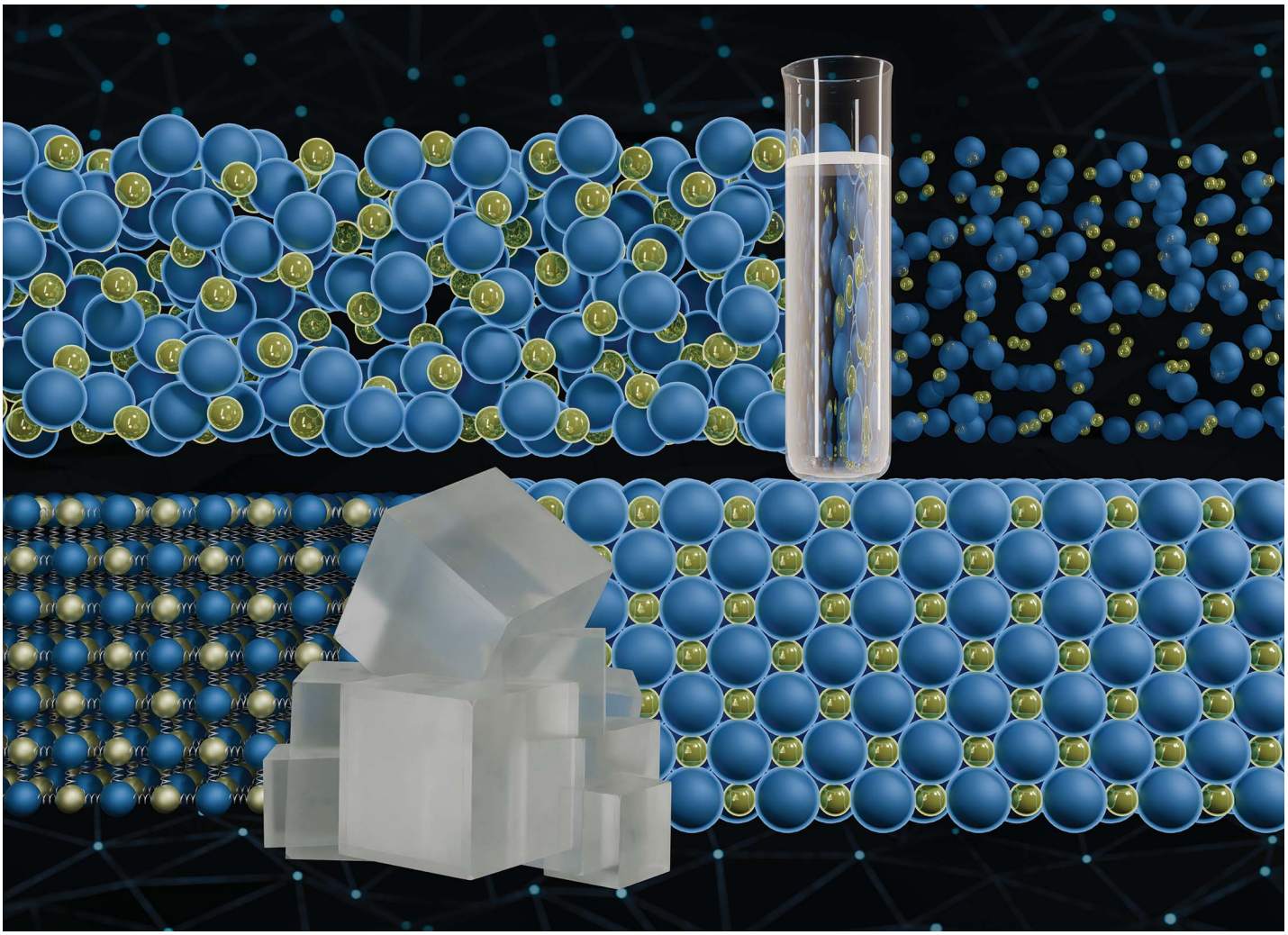

Showcasing research from Dr. Luke D. Gibson, Dr. Rajni Chahal, and Dr. Vyacheslav S. Bryantsev at Oak Ridge National Laboratory, Oak Ridge, TN, USA.

Computing chemical potentials with machine-learning-accelerated simulations to accurately predict thermodynamic properties of molten salts

Machine learning interatomic potentials are used to accelerate free energy calculations in an efficient framework for computing chemical potentials without a loss in accuracy compared to DFT. The effectiveness of this general framework is demonstrated by predicting the melting point of lithium chloride from solid- and liquid-phase chemical potentials computed at multiple temperatures. By developing this capability to accurately and efficiently evaluate chemical potentials, this work provides the means for predicting thermodynamic properties with quantum chemical accuracy that would otherwise be difficult to compute, such as redox potentials, phase diagrams, and solubilities.

As featured in:

See Luke D. Gibson, Vyacheslav S. Bryantsev *et al.*, *Chem. Sci.*, 2025, **16**, 3078.

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