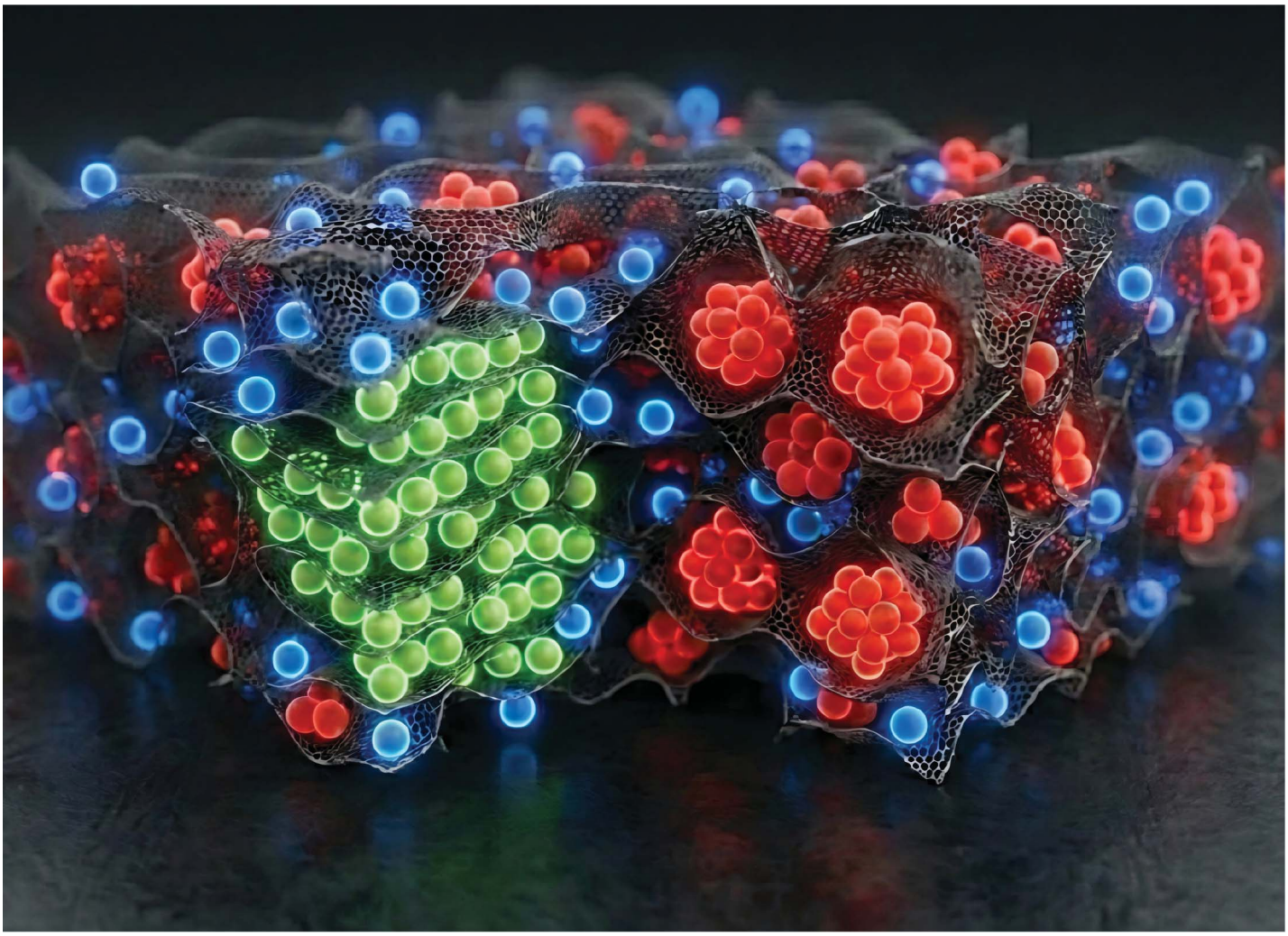

Showcasing collaborative research from Professor Xiao Wang and Professor Feng Ding, Suzhou Laboratory, Suzhou, China.

Unveiling sodium storage mechanisms in hard carbon *via* machine learning-driven simulations integrated with accurate site occupation identification

Hard carbon (HC) has attracted considerable interest as a promising anode material for sodium-ion batteries (SIBs). Nevertheless, the sodium storage mechanism in HC remains poorly understood owing to challenges in precisely characterizing its structure. Xiao Wang and co-workers unveils atomic-scale sodium storage mechanisms in HC via machine learning-driven simulations. By integrating a neural network potential with random forest site identification, contributions from adsorption, intercalation, and pore-filling sites were quantitatively disentangled. This work accurately correlates specific storage sites with voltage and capacity, providing a computational framework for investigating SIB anodes.

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Artwork generated in part using Google Gemini.

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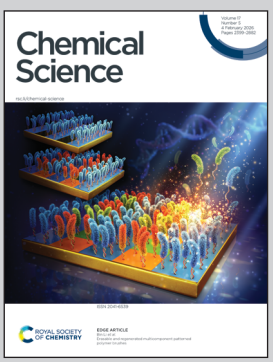

See Feng Ding, Xiao Wang *et al.*, *Chem. Sci.,* 2026, **17**, 2547.

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