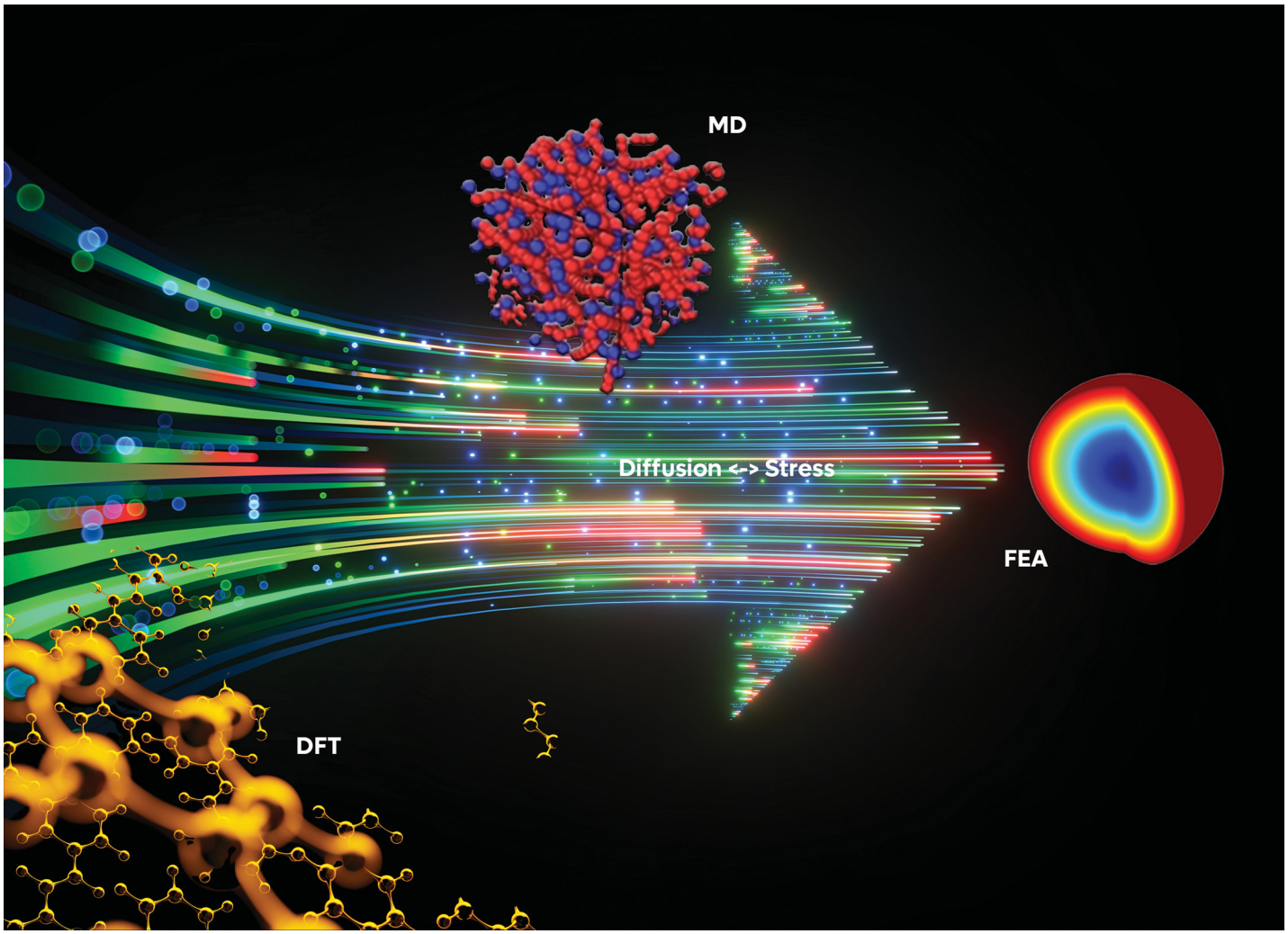

Showcasing research from the group of Prof. Tarun Kumar Kundu at Indian Institute of Technology, Kharagpur, India.

A comprehensive diffusion-induced stress coupled multiscale modeling and analysis in hard-carbon electrodes of Li-ion batteries

A comprehensive multiscale approach is proposed to optimize the particle size by studying the diffusion-induced stress (DIS) in hard carbon (HC) particles as the potential anode material for high-energy LIBs. Density functional theory is used to calculate state of charge (SOC) dependent coefficient of volume expansion. SOC dependent diffusivity and elastic modulus are calculated *via* molecular dynamics. These results are used in continuum model to examine the concentrations and DIS in HC particles lithiated at various C-rates.

As featured in:

See Tarun Kumar Kundu *et al.*, *Phys. Chem. Chem. Phys.*, 2023, **25**, 20462.

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