Exploring Energy Materials via Hybrid Modeling: Atomic, Continuum-scale, and Machine Learning Potentials

Hong-Kang Tian[1,2,3,*]

[1] *Department of Chemical Engineering, National Cheng Kung University, Tainan 70101, Taiwan;*
[2] *Program on Smart and Sustainable Manufacturing, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 70101, Taiwan;*
[3] *Hierarchical Green-Energy Materials (Hi-GEM) Research Center, National Cheng Kung University, Tainan 70101, Taiwan*

Email address of the corresponding author: hktian@gs.ncku.edu.tw

Advancing next-generation energy materials requires a deep, atomistic understanding of their structural and transport properties. This talk presents a multi-scale modeling approach—combining *ab initio* DFT, DFT-based Molecular Dynamics (DFT-MD), Finite Element Analysis (FEA), and Machine Learning Interatomic Potentials (MLIPs)—to address key challenges in battery and catalytic materials. For all-solid-state batteries, we investigate the dual influence of protonation and doping on Li-ion transport in garnet-type LLZO electrolytes[1,2] and use FEA to model internal stress, interfacial contact, and composite cathode behavior. We further explore interfacial effects on dendrite formation in Li and Mg anodes, revealing the critical role of SEI composition in stability[3]. In catalytic materials, our simulations guide the design of high-performance catalysts, including Co-Fe Prussian blue analogs for water oxidation and Fenton-like reactions[4] and Ni-Fe spin-polarized 2D π-d conjugated frameworks for oxygen evolution reactions[5]. Finally, we employ DFT and MLIPs to reveal and optimize the phase stability of lead-free Sn-based perovskites $FA_xMA_{1-x}SnI_3$.[5] By integrating multi-scale simulations with MLIPs, we provide insights into doping, interfacial engineering, and catalytic activity, accelerating the development of efficient and sustainable energy materials.

References

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