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ABSTRACT

Advancing Bioinspired and Low Dimensional Composite Materials Through High-Accuracy Simulations

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The simulation of bioinspired materials and hierarchical assembly of building blocks for molecular recognition, electrical, and mechanical functionality is essential for advancing sensor and structural applications. Computational and AI-driven methods accelerate progress, and this work highlights molecular dynamics (MD) simulations of the recognition of peptides, biomolecules, and polymers on 2D materials such as MXenes, MoS_2, and metal-organic frameworks (MOFs). Molecular mechanisms of assembly, binding energies, and mechanical properties up to failure are illustrated using molecular simulations in beyond-DFT accuracy. We describe how to achieve exceptional reliability, speed, and compatibility among common simulation platforms using the INTERFACE force field (IFF) and reactive INTERFACE force field (IFF-R). We discuss how understanding from MD simulation as well as through AI/ML can be integrated with findings from experiments (scattering, imaging/microscopy, spectroscopy, binding assays, calorimetry). The critical role of crystallographic facets, electrolyte composition and pH values will be highlighted, which is often elusive or less regarded in experiments.