Modeling Self-assembled Hydrogel Scaffold for Hydrogen Generation

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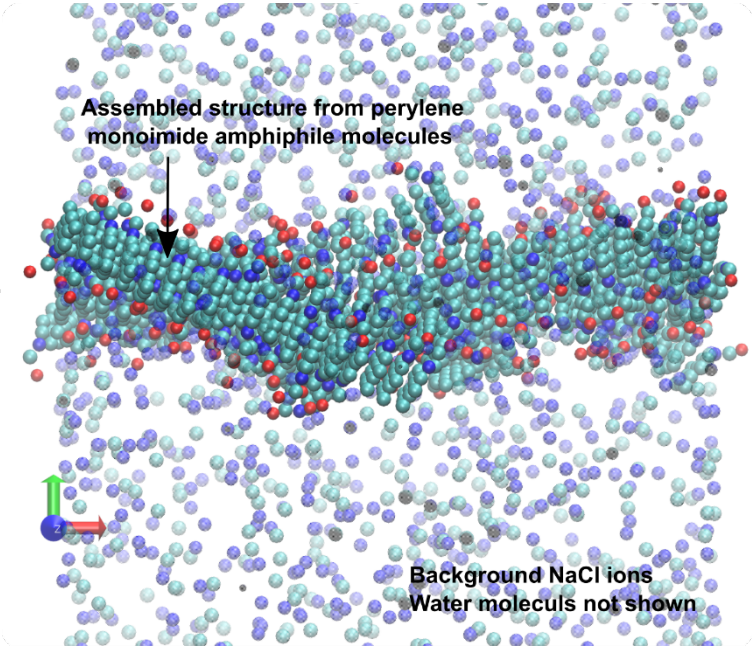
Supramolecular self-assembly systems had enormous opportunities in energy-related applications. However, the structures and dynamics were not always understood. In a collaboration between Olvera lab and Stupp lab under NU MRSEC Superseed, one perylene monoimide amphiphile based self-assembly system was investigated. The system formed finite-width nano-ribbons, which evolved into a hydrogel scaffold. The scaffold proved to be a suitable host for catalytic hydrogen generation. Multiscale molecular dynamics simulations, together with analytical and numerical modeling were constructed for analysis. The width and the shape of the ribbons were correlated with the molecule's inherent molecular interactions and the strength of external dielectric environment.



Snapshot of the Coarse Grain Simulations

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