

Elucidating the aromatic properties of covalent organic frameworks surface for enhanced polar solvent adsorption

ABSTRACT

Covalent organic frameworks (COFs) have a distinguished surface as they are mostly made by boron, carbon, nitrogen and oxygen. Many applications of COFs rely on polarity, size, charge, stability and hydrophobicity/hydrophilicity of their surface. In this study, two frequently used COFs sheets, COF-1 and covalent triazine-based frameworks (CTF-1), are studied. In addition, a theoretical porous graphene (TPG) was included for comparison purposes. The three solid sheets were investigated for aromaticity and stability using quantum mechanics calculations and their ability for water and ethanol adsorption using molecular dynamics simulations. COF-1 demonstrated the poorest aromatic character due to the highest energy delocalization interaction between B–O bonding orbital of sigma type and unfilled valence-shell nonbonding of boron. CTF-1 was identified as the least kinetically stable and the most chemically reactive. Both COF-1 and CTF-1 showed good surface properties for selective adsorption of water via hydrogen bonding and electrostatic interactions. Among the three sheets, TPG's surface was mostly affected by aromatic currents and localized π electrons on the phenyl rings which in turn made it the best platform for selective adsorption of ethanol via van der Waals interactions. These results can serve as guidelines for future studies on solvent adsorption for COFs materials.

Keyword: Covalent organic frameworks; COF-1; CTF-1; Aromaticity; Stability; Water; Ethanol