

Beyond the Surface: How Electronic Structure Controls Adsorption in 2D Organic Nanomaterials

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Abstract :

Two-dimensional (2D) carbon-based materials offer precise control over adsorption, yet the governing electronic principles remain incompletely understood. In this talk, I will present integrated insights from pollutant adsorption, heteroatom tuning, interlayer twist engineering, and ion-surface interactions. Using density functional theory (DFT), we reveal how π -surface chemistry, nitrogen substitution, and layer topology collectively control binding strength, charge redistribution, and orbital reorganization. Across N-doped COFs, twisted COF bilayers, and graphane interfaces, a unified principle emerges: adsorption is governed by local electronic symmetry, heteroatom-induced polarity, and tunable π - σ coupling. Additional analyses highlight how defects, substituents, and interlayer registry alter adsorption geometries and stabilize preferred configurations. Energy-decomposition results clarify the relative roles of dispersion, electrostatics, and weak charge transfer. These results establish generalizable design rules for sensing, molecular recognition, and reactivity control in emerging 2D organic nanomaterials.

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学術変革領域研究(B)
スケール横断分析
Cross-scale Analysis

