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Molecular Dynamics of a Series of Self-Assembling Organic Monolayers: Selective Adsorption and Catalysis on 2D Molecular Sieves
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Spontaneous molecular self-assembly is a promising route for bottom-up manufacturing of two-dimensional (2D) nanostructures with specific topologies on atomically flat surfaces. Of particular interest is the possibility of selective lock-and-key interaction of guest molecules inside cavities formed by complex self-assembled host structures. Our host structure is a monolayer consisting of interdigitated 1,3,5-tristyrylbenzene substituted by alkoxy peripheral chains containing $n = 6$, 8, 10, 12, or 14 carbon atoms (TSB3,5-Cn) deposited on a highly ordered pyrolytic graphite (HOPG) surface. Using *ab initio* methods from quantum chemistry and molecular dynamics simulations, we construct and analyze the structure and functionality of the TSB3,5-Cn monolayer as a molecular sieve. Supported by ACS-PRF 52696-ND5.

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