Abstract Submitted
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Self-Assembly and Dynamics of Organic 2D Molecular Sieves: *Ab Initio* and Molecular Dynamics Studies[1] ALEXANDER ST. JOHN, CARLOS WEXLER, Univ of Missouri - Columbia — 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.

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