Self-Assembly and Dynamics of Organic 2D Molecular Sieves: Ab Initio and Molecular Dynamics Studies 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-C\( n \)) 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-C\( n \) monolayer as a molecular sieve.

1Supported by ACS-PRF 52696-ND5