

Abstract Submitted  
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**Computational**

**Study of Supramolecular Self-Assembly Using CH/ $\pi$  Bonds**

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P. MAKSYMOWYCH, M. PAN, CNMS, ORNL — Self assembly is an

important research area in supramolecular engineering. We show that CH/ $\pi$  bonds can be exploited as a vehicle to assemble clusters of well-defined sizes on metal surfaces. Specifically, we theoretically explain the observations of largely uniform distribution of phenylacetylene magic clusters, each consisting of six molecules, on Au(111) surfaces. Using density functional theory with a van der Waals functional, we discuss the reasons for the preference of the hexamer structure, the key effect of CH/ $\pi$  bonding on the self-assembly, and the critical role of the metal surface. Our calculated STM images and electronic properties are in good agreement with experiment. The cooperative, multi-center CH/ $\pi$  interactions offer an attractive tunability via chemical functionalization, and thus may provide a new avenue towards rationally designing a desired supramolecular shape and size.

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