Abstract Submitted
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Understanding the growth of organic semiconductors on semiconducting surfaces MINA YOON, CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, BING HUANG, Beijing Computational Science Research Center, SEAN R. WAGNER, PENGPENG ZHANG, Michigan State University — A selective mechanism for tuning the molecule-substrate interaction has been a long sought after goal towards tailored molecular growth. Using first-principles theory and scanning tunneling microscopy, we show that by controlling the strength of orbital hybridization between phthalocyanine molecules and the deactivated Si surface via the selective p-d orbital coupling, we can tune the molecular ordering and molecular orientation at the hetero-interface. This mechanism offers a novel approach to balance the critical interactions, leading to controlled long-ranged ordered molecular growth [1]. [1] S.R. Wagner, B. Huang, C. Park, J. Feng, M. Yoon, and P. Zhang, Phys. Rev. Lett. 115, 096101 (2015). This work was supported by the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy and partly supported by the Materials Sciences and Engineering Divisions, Office of Basic Energy Sciences, U.S. Department of Energy.

Mina Yoon
Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

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