Abstract Submitted
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Tailored Organic Molecular Growth on Silicon Studied by STM and DFT* SEAN WAGNER, Michigan State University, BING HUANG, CHANGWON PARK, Oak Ridge National Laboratory, JIAGUI FENG, Michigan State University, MINA YOON, Oak Ridge National Laboratory, PENGPENG ZHANG, Michigan State University — Control of highly ordered organic molecular thin films with extended π systems is currently of intense interest for integrating molecules into modern electronics due to their tunable nature. Selection of molecules and substrates can lead to desired transport properties such as charge transfer, charge injection, exciton diffusion, etc., at the hetero-interface, which is crucial to the development of organic and molecular electronics. Combining scanning tunneling microscopy and density functional theory, we show that by appropriately choosing the coordinated transition-metal ion in metal phthalocyanine, the strength of the molecule-substrate interaction can be tailored, allowing for the molecular ordering and orientation at the hetero-interface with the silicon substrate to be tuned accordingly. This mechanism provides new control over the delicately balanced molecule-substrate and intermolecular interactions, offering a route towards well-ordered organic molecular growth. *Experimental work is funded by the U. S. DOE Office of Science Early Career Research Program (DE-SC0006400) through the Office of Basic Energy Sciences. Theory work conducted at Oak Ridge National Laboratory is sponsored by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. DOE.

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