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Dispersion Forces and Self-assembly of Styrene Nanowires on H-Si(100) 2×1 Surface[1] GUO LI, Institute of Physics, CAS, P. R. China; U of Tennessee at Knoxville, VALENTINO COOPER, Oak Ridge National Laboratory, JUN-HYUNG CHO, Hanyang University, Korea, SHIXUAN DU, HONGJUN GAO, Institute of Physics, CAS, P. R. China, ZHENYU ZHANG, Oak Ridge National Laboratory; U of Tennessee at Knoxville — We present our first-principles investigation of the influence of dispersion forces (or van der Waals interactions) on the self-assembly of styrene nanowires on the hydrogenated Si(100) 2×1 surface. Using density functional theory (DFT) calculations and kinetic Monte Carlo (KMC) simulations we demonstrate that the dispersion forces enhance the binding between styrene molecules thus allowing us to tune the preferential growth of long wires for the fabrication of desired nanopatterns. Furthermore, this approach is a step towards accurate fully first-principles studies of the effects of dispersion forces on the dynamics at interfaces, and therefore will be invaluable to our understanding of chemical processes such as self-assembly and the catalysis of organic chemical reactions.

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