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High-Throughput Screening of Substrates for Synthesis of Two-Dimensional Materials ARUNIMA K. SINGH, NIST - Natl Inst of Stds & Tech, HOULONG L. ZHUANG, Oak Ridge National Laboratory, FRANCESCA TAVAZZA, NIST - Natl Inst of Stds & Tech, RICHARD G. HENNIG, University of Florida, Cornell University — Since the discovery of graphene, several two-dimensional (2D) materials have been synthesized experimentally, but many theoretically predicted 2D materials are yet to be synthesized. Common synthesis techniques such as chemical-vapor deposition and molecular-beam epitaxy require suitable substrates. We are developing a strategy to enable high-throughput searches for suitable substrates for 2D materials by automatically identifying suitable substrate candidates and characterize their stabilizing properties and doping effects using density-functional theory. As first steps, we have found that several transition-metal, rare-earth-metal, and refractory-diboride substrates sufficiently reduce the formation energies of 2D group-III-V materials, making them thermodynamically stable on these substrates [1,2]. Additionally, these substrates lead to variable amount of doping of the 2D materials depending on the work functions of the 2D materials and the substrates. We observe large adsorption energies and strong doping of the 2D materials which indicates that these substrates can provide good electrical contact to enable transport measurements and electronic applications.

[1] Physical Review B 89 (24), 245431 (2014).

[2] Applied Physics Letters 105 (5), 051604 (2014).

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