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Abstract for an Invited Paper
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Computational Discovery, Synthesis, and Functionalization of 2D Materials[1]

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Less than 5 % of the >6000 theoretically predicted and promising two-dimensional (2D) materials have been experimentally synthesized. In this talk, I will present a density-functional theory based framework that can be used to identify suitable substrates that enable growth and functionalization of as-yet-hypothetical 2D materials. We have applied this formalism to identify substrates for 2D group-III-V materials, validated it against experimental synthesis of 2D MoS_2 and integrated the results from the framework with phase-field models to predict the micro-structure of graphene on various metallic substrates. We are currently applying this strategy for a high-throughput screening of substrates for the thousands of as-yet hypothetical 2D materials. In order to automate the steps associated with the search such as generation of heterostructures, creation of input files, submission of runs on computing resources, post-processing of simulations, error management and curation of key properties in an open-source database, we have developed open-source python-packages. The high-quality electronic structure data and physio-chemical properties of 2D materials-substrate interface emerging from this study will provided an invaluable theoretical input to 2D materials growers as well as serve as a critical atomic-scale input for multi-scale studies leading to an accelerated growth and functionalization of 2D materials.

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