University of Crete
Department of Physics

Physics Colloquium

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Towards the computational design of Moire assemblies

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ABSTRACT

Fostering innovation in nanotechnology relies on the continuous development of nanostructures with exceptional properties as active materials. Graphene and other two-dimensional (2D) materials such as transition metal dichalcogenides constitute structurally simple, but nevertheless fascinating, examples of materials that could redefine information processing, energy storage, and a host of other technologies. Although some single- and few-layer forms of these materials have been realized and thoroughly studied, the space of arbitrarily layered assemblies remains mostly unexplored.

I will present theoretical concepts, materials models, and computational methods towards an automated virtual lab for the investigation of the electronic structure of layered materials, and the exploration, as an application, of the spaces of two-layer molybdenum disulfide, multi-layer graphene, and model one-dimensional layered assemblies. This work more generally combines physics-based and data-driven approaches to demonstrate precise control of the electronic properties of layered materials through guided choice of the constituent layers, their stacking, and relative orientation, with important implications for the development of novel devices.

[1] A. K. Geim and I. V. Grigorieva, Nature 499, 419 (2013).

[2] G. A. Tritsaris, S. Carr, G. R. Schleder, P. Protopapas, E. Kaxiras, https://arxiv.org/abs/2011.04795