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Atomistic Control of the Dynamical Electronic Properties of 2D Materials and Beyond[1]

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Two-dimensional (2D) materials, such as graphene, transition metal dichalcogenides and recently found 2D-perovskites, have attracted intense interest for their fascinating electronic properties, and exhibit strikingly different optoelectronic and mechanical features from their 3D-bulk counterparts. They are promising for a wide range of applications, including flexible, mechanically strong electronics such as transistors, memories, logic circuits, light emitters and photodetectors. In this presentation I will discuss different alternatives ranging from electric fields, strain, Ar-plasma treatment, to synthesis processes, to precisely control intrinsic material properties. I will describe several case studies where the synergy between in-silico predictions and experiments has driven smart devices with novel set of functional chemical and physical properties. Moreover, I will discuss some challenges at the forefront of 2D-perovskite materials as the few-layer limit is reached and new device-platforms for energy conversion applications.

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