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Doping Dependent Electronic Properties of Atomically Thin Two-dimensional Crystals¹ TING CAO, ZHENGLU LI, STEVEN G. LOUIE, Physics Department, UC Berkeley and Lawrence Berkeley National Lab — Using first-principle calculations, we find that the electronic structure of atomically thin 2D crystals such as GaSe and NbSe2 can be modified significantly through doping, which can lead to major changes in their other properties. We elucidate the origins of these doping dependent effects, and connect our theoretical predictions to experimental measurements since high level of doping can be achieved in 2D materials.

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