Intrinsic point defects inside the monolayer of TMDs from first-principles calculations

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Abstract

Besides Graphene, there is a zoo of materials which can be synthesized to a two-dimensional (2D) layer [1]. Among which, transition metal dichalcogenides (TMDs) have shown promising applications in field effect transistors, flexible devices, optoelectronics, and many more [2]. Due to thermodynamical conditions, crystalline defects are usually present in materials which, in turn, change their properties. Moreover, these 2D materials resist inelastic relaxations up to an enormous fraction of their ideal strength yet it is possible to tune their band gap via strain [3]. Thus, strain engineering of these 2D materials is proposed and investigated. In this talk, I will go over the effect of compressions and tensions on the energetics, electronic, and optical properties of TMDs monolayer containing intrinsic defects. I have studied point vacancies and some substitutions.

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