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First principal study of stability, structural and electronic properties of 1T(2H)-NbS_2 and Ni doped 1T(2H)-NbS_2

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Abstract:

Lamellar dichalcogenides constitutes approximately two thirds of transition metals dichalcogenides TMX_2 (TM= Transition Metal and X= S, Se or Te) listed in the literature. In the 1970's and 1980's, they gave rise to numerous studies. These compounds possess a strong anisotropy: strong connections within the layers and weaker interactions, van der Waals type, assuring the link between these layers. One of the direct consequences of such a structural organization is the possibility of realizing splits, of obtaining properties of lubrication or of observing physical anisotropic properties. One of the most interesting points in the family of lamellar dichalcogenides lies in the possibility of inserting ions between layers, or even more or less complex molecules.
Disulfides TMS_2 are a part of this big family of lamellar dichalcogenides: they crystallize mainly in octahedral (1T) and trigonal (2H) with space groups $P\bar{3}m1$ (164) and $P6_3/mmc$ (194) respectively. These phases are mostly characterized by the occupation of one half of spaces between the anionic layers.
In this work, we calculate the structural and electronic properties of Ni doped NbS_2 and NbS_2. This to understand the nature of the chemical connections, the effect of doping by Ni and the origin of the structural order existing in NbS_2. Calculation is made via ab-initio Ultra-soft pseudo-potential calculations within density functional theory (DFT).
Keywords:
Abinitio, anisotropy , Dichalcogenides of transition metals TMX_2, 1T and 2H phases.