Composition Dependence of the Charge Driven Phase Transition in Group-VI Transition Metal Dichalcogenides

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Abstract

The experimental exfoliation of transition metal dichalcogenates (TMD) frequently involves a step involving alkali ion intercalation. This intercalation is known to induce structural phase transitions in Group-VI TMDs from a semi-conducting H-phase to a metallic T' - phase. However, this rate at which this occurs is known to be composition dependent, with higher amounts of H'-phase present in WS_2 compared to MoS_2 [1].

This phase transition can be exploited for various applications such as transistors, sensors and catalysis. However, it is difficult to experimentally decouple the effect of composition-dependent energy barriers from indirect effects related to alkali metal-induced exfoliation [2].

Here we use density functional theory calculations for group-VI TMDs (MX_2, where M = Mo, W and X = S, Se) to study the effect of adsorbed alkali metal ion on the energetics of the transition process [3]. The calculations show that the higher proportion of H phase in MoS_2 can be explained by the higher barrier for transition on alkali metal ion adsorption. Likewise, the high proportion of metallic phase in WS_2 monolayers after alkali treatment can be explained by a high barrier to revert back to the H phase once in a neutral state. We also discuss the lowering of transition barriers for reverse conversion from T' to H phase via the formation of intermediate mixed phase [4].

References

[1] Voiry et al, Chemical Society Reviews 44, 2015, 2702
[2] Ambrosi et al, Chemical Communications, 51, 2015, 8450
[3] Patil et al, arXiv:1901.02697v1 [cond-mat.mtrl-sci]
[4] Ma et al, N*anoscale 8, 2016, 4969*

Figures

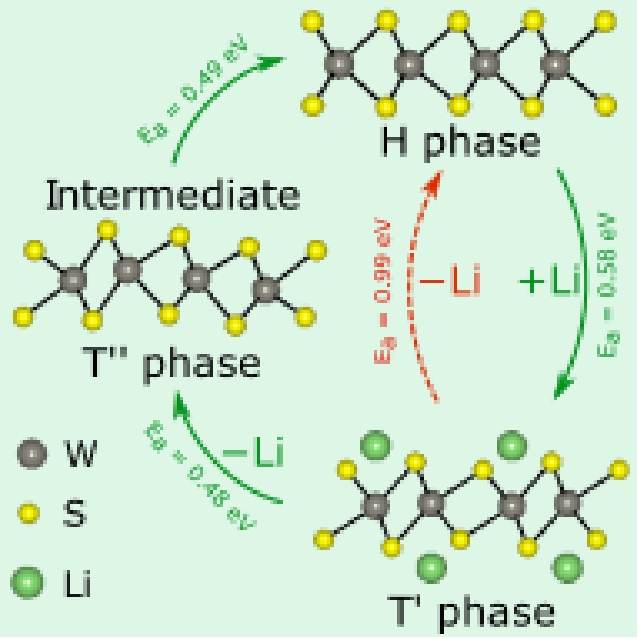

Figure 1: Flow diagram for transition of WS2 showing the reverse conversion via an intermediate mixed phase