**First-Principles Study of Alkali Metal Intercalated MoS2**

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MoS2 is a compound in transition metal dichalcogenide (TMDC) family that is semiconductor with layered honeycomb structure having strong in-plane bonding and weak out-of-plane van der Waals interactions. In the bulk form, MoS2 has an indirect band gap, whereas monolayer form has direct band gap which is more suitable for device applications. It has been proposed that the electronic characteristic of the monolayer can be reproduced experimentally in MoS2 by K intercalation [1]. In this work, the effects of different alkali metal (such as Li, Na, K, and Rb) intercalation are investigated by using first-principles calculations within the 2×2×1 supercell. In order to provide guidance for measurement, the electronic structures from supercell calculations are unfolded onto the high symmetry paths [2] as defined in the first Brillouin zone of the primitive cell. The results show significant expansion of interlayer spacing and contribution of electron donation from alkali metal to the conduction band of MoS2. The expansion obviously depends on atomic radii of the intercalated metals. Moreover, the conduction band minimum is changed to the same location of the valence band maximum in *k*-space because the expansion of the interlayer spacing reduces the electronic interactions between adjacent layers creating a quasi-monolayer character. It has been found that the interlayer spacing of MoS2K0.25 and MoS2Rb0.25 are large enough to exhibit quasi-monolayer character. Furthermore, the effects of concentration of alkali metal have been investigated by varying concentration of K within the given supercell. We found that in-plane lattice constant increases proportional to the concentration. Our results suggest that different atomic radii and concentration of intercalated alkali metals could provide an opportunity to tune electronic structures of TMDC materials.

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2. M. Tomić, H. O. Jeschke, and R. Valentí, Phys. Rev. B **90**, 195121 (2014).