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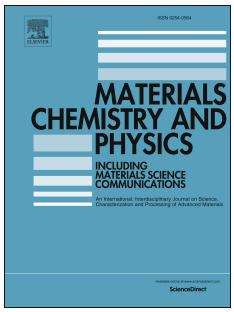


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# Influence of Mo-vacancy concentration on the structural, electronic and optical properties of monolayer $MoS_2$: A first-principles study

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**Abstract:** Effects of Mo-vacancy concentration on the structural, electronic and optical properties of monolayer $MoS_2$ have been investigated using the first-principles calculations. Results show that Mo-vacancy is prone to form in monolayer $MoS_2$ under S-rich condition. S atoms around Mo-vacancy exhibit an outward relaxation, whereas Mo atoms around Mo-vacancy show an inward relaxation. At low Mo-vacancy concentration, some localized impurity states are induced in the band gap of monolayer $MoS_2$, coupled with a band gap increment. As the Mo-vacancy concentration increases, the impurity states become delocalized and mix with the upper valence bands, resulting in the band gap decrease. The covalent character of Mo-S bonding is enhanced upon the introduction of Mo-vacancy, and the enhancement is weakened as the Mo-vacancy concentration increases. Optical properties calculations show that the static dielectric constant increases with the increasing Mo-vacancy concentration. The imaginary part of complex dielectric function exhibits a little blue shift for monolayer $MoS_2$ with low Mo-vacancy concentration, whereas the imaginary part of complex dielectric function shows distinct red shift for monolayer $MoS_2$ with high Mo-vacancy concentration.

**Keywords:** Monolayer $MoS_2$; Mo-Vacancy; Vacancy concentration; First-principles

## 1. Introduction

Transition-metal dichalcogenides (TMDs) have attracted wide attention because of their potential applications in next-generation nano- and opto-electronic devices. Monolayer $MoS_2$, one of two-dimensional TMDs, has drawn great interest due to its atomically thickness of ~7 Å [1],

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