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Tuning electronic and magnetic properties in monolayer MoSe₂ by metal adsorption

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Abstract

We have systematically explored the electronic structures and magnetic properties of metal Pd, Pt, Cu, Ag, Au and Zn adsorbed MoSe₂ monolayer by means of first-principles calculations. It reveals that stable chemical adsorption has been formed between the adatoms Pd, Pt, Cu, Ag, Au and MoSe₂ monolayer, however, weak physical interaction is found between Zn and MoSe₂ monolayer owing to the small adsorption energy. Both the framework structure and electronic property of the metal adsorbed MoSe₂ monolayer are slightly tuned by the adatoms. More importantly, magnetic character is introduced in Cu, Ag and Au systems.

Keywords: MoSe₂ monolayer; metal adsorption; electronic and magnetic properties; First-principles calculations

1. Introduction

Since the discovery of graphene in 2004, two-dimensional layered materials have inspired a surge of interests [1-3]. Among them, layered transition-metal dichalcogenides (LTMDs) have attracted a great deal of attention owing to their

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