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ABSTRACT

Using first principles calculations, we have investigated the pressure effects on the electronic and optical properties of Tungsten Disulfide. The results show that the lattice out plane is more sensitive to the pressure than that in plane. In addition, the conduction band maximum drops down and the valence band minimum shifts up with respect to the Fermi level, respectively. Semiconductor to metal transition occurs at a critical pressure(~36Gpa). Moreover, the dielectric function also has an obviously red shift, and the optical absorption can be improved accordingly. Our study supplies a route to optimize the performance of WS_2 devices.

1. Introduction

Transition metal dichalcogenides (TMDs) are layered materials similar to graphite, in which the covalent bonded layers are weakly coupled by van der Waals (vdW) interactions. TMDs such as layered MoS_2 and WS_2 have attracted intensive attentions due to the distinctive and varied properties, which suggest potential applications in the areas of electronic and optoelectronic devices [1-3]. Recently, the pressure effects on TMDs have attracted great interests in various fields, i.e., mechanics, optics, and electronics [4-6]. Hydrostatic pressure without inducing impurities provides an easy but powerful tool, to modulate the geometrical and electronic structures, and improve the performance of TMDs based devices consequently.

For bulk MoS_2, it has been both experimentally and theoretically found that the pressure can not only induce a transition from semiconductor to