Ab initio study of the energy loss near sulfur K and L$_{2,3}$ edges of layered MS$_2$ (M = Ta, Nb and V) in trigonal prismatic and octahedral structures

Mehrdad Dadsetani*, Tahereh Nouri, Hajar Nejatipour

Department of Physics, Lorestan University, Khoramabad, Iran

ARTICLE INFO

Article history:
Received 24 October 2016
Received in revised form 11 March 2017
Accepted 11 March 2017
Available online 14 March 2017

Keywords:
Transition metal disulfide monolayers
Trigonal (2H) and octahedral (1T) phases
Sulfur K and L$_{2,3}$ edge
Density functional theory
Core-hole approximation

ABSTRACT

This study set out to calculate the full-potential linearized augmented plane wave (FPLAPW)-based energy loss near sulfur K and L$_{2,3}$ edge structures of group V transition metal disulfides MS$_2$ (M = Ta, Nb, and V) in octahedral (1T) as well as trigonal prismatic (2H) structures. The calculations showed that, consistent with other calculations, all the studied materials were metallic due to the partially filled d bands in their configurations. Furthermore, the calculated ELNES spectra revealed a good agreement with the available experimental XANES analogues. The d-like and p-like transitions of M and sulfur atoms were the dominant electron transitions in K edge spectra. Spectrum characteristics of the sulfur L$_{2,3}$ edge of ELNES indicated the transition of sulfur-p electrons to the unoccupied s or d states. These spectra reflect the electronic band structures of materials, as well. As the focus shifts from bulk to monolayer, substrate hybridization becomes stronger. In 2H phases, the dominant peaks of sulfur K edge spectra originate from unoccupied d bands. Further, the broad peaks at higher energy ranges are due to the transitions to sulfur p hybridized with M-s and p states. For energies below 7 eV, M-d state is the target state of most of the transitions in both 1T and 2H phases. For above 10 eV energies, however, sulfur-d is the target state. Moreover, density of states of sulfur-p (d) is very similar in shape to that of sulfur K (L$_{2,3}$) edges spectra. For the sulfur L$_{2,3}$ edges, from 2H-TaS$_2$ to 2H-VS$_2$ and also from bulk to monolayer, the number of transitions to M-d state increases.

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1. Introduction

The group V layered transition metal disulfides (LTMDSs) with the formula MS$_2$ (M = Nb, Ta and V) have attracted a lot of interest due to the recent developments in sample preparation, optical detection and manipulation of two-dimensional materials. Layered structures of these materials have the form S-M-S with the transition metal atoms (M) sandwiched between two separated planes of sulfur atoms. Their two-dimensional nature is because of the weak bonding between the adjacent sheets which are held together by van der Waals forces. The weak bonding is considered for making lubricants, doing catalysis, conducting photo and electro-catalytic hydrogen reactions, and developing ultrasensitive moisture responsive devices (Mattheiss, 1973b; Wilson and Yoffe, 1969; Radisavljevic et al., 2011; Coehoorn et al., 1987; Docherty et al., 2014; Feng et al., 2012). VS$_2$ can provide some basic principles to enhance lithium interaction and diffusion, and to develop new lithium-ion battery materials. VS$_2$ intercalated with lithium can be a highly promising 2D anode material with excellent electrochemical performances. With its metallic nature, VS$_2$ monolayer is a suitable electrode material for Li-ion batteries, super capacitors and solar cells. TaS$_2$ is observed in both octahedral (1T) and trigonal prismatic (2H) structures, while NbS$_2$ and VS$_2$ are respectively crystalized in 2H and 1T phases. Scholars have widely investigated NbS$_2$, TaS$_2$, and VS$_2$ materials to identify their properties. Linear muffin tin orbital method shows significant anisotropy in the frequency-dependent dielectric function of 1T-TaS$_2$ (Sharma et al., 2000). Studies show that tensile strain magnetizes the layered NbS$_2$ with a ferromagnetic quality (Zhou et al., 2012). Scanning tunneling microscopy verifies the peculiar superconducting density of states of 2H-NbS$_2$ (Guillamón et al., 2008). Another finding is that highly conductive VS$_2$ thin films are very useful for constructing the electrodes of in-plane supercapacitors (Feng et al., 2011). Analysis of electrical properties of TaS$_2$ shows that increasing the temperature leads to transitions between the semiconducting and metallic...