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LITHIUM/SODIUM EFFECTS ON THE STRUCTURAL AND ELECTRONIC PROPERTIES OF TITE2 MONOLAYERS FOR BATTERIES

The demand for portable electrical energy is growing due to the use of mobile devices which satisfy daily needs. In that context the dichalcogenide TiTe2 has demonstrated a charging voltage of ~ 0.7 V (Zn2+/Zn) and a reversible capacity of 225 mAh/g [1]. Currently, it has been possible to synthesize the 1T-TiTe2 monolayer [2]. In this work, a systematic study was made of the Li/Na effect on the TiTe2 monolayer in the different adsorption-sites on the structural and electronic properties; This was carried out using DFT implemented in the CASTEP code. Structural properties show increments for the monolayers in lattice parameters a and b due to the insertion of Li/Na in the different adsorption-sites. Besides, it is observed that the Top- and Hollow-sites could be the most stables for adsorption of Li/Na atoms. Furthermore, the electronic properties for the TiTe2 bulk compound and Pristine monolayer shows a metallic behavior in the similar way for the monolayers with Li/Na on the different adsorption-sites. This behavior is due to the interaction of *p*-Te and *d*-Ti orbitals. Finally, the voltage obtained indicates that this material can be used as an anode in ion batteries.

Keywords

Batteries, TiTe2, DFT, Monolayers, Electronic properties.

Reference

[1] Y. Du, et al., J Mater Chem A Mater 10 (2022) 16976–16985. [2] P. Chen, et al., Nat Commun 8 (2017) 516.

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