

Alkali metal diffusion on low-density 2D structures

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Transition metal dichalcogenides (TMD) are a promising class of two-dimensional materials for use as materials for energy storage characterized by a high capacity [1]. At the moment, in order to increase the efficiency of these materials, new phases and classes are being synthesized [2]. The features of alkali metal (Li and Na) diffusion on the surface of novel 2D low-density MoX₂ (X = S, Se) structure were investigated. This structure was obtained by the method for searching of random structures—Ab initio Random Structure Searching (AIRSS) and is interesting in terms of comparing its physical properties with the already synthesized octahedral (1T) and trigonal-prismatic (2H) phases [3]. The stability of this phase was determined by an investigation of the phonon spectra. The migration barriers of alkali atoms were determined by the NEB method. Based on barrier values the intercalation voltage was calculated.

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