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Relative stability of octahedral and trigonal prismatic phases of MoSe2 flakes from density functional theory calculations

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Nowadays, transition metal dichalcogenides (TMDs), materials with chemical formula MQ_2 (M = transition metal; Q = S, Se, Te), are among the most promising two-dimensional materials, being widely studied due to the unique physical properties and phenomena they exhibit. (1-2) Each layer in a TMD crystal structure is composed by one plane of M atoms sandwiched between two planes of Q atoms, and two different coordination environments, namely, trigonal prismatic (1H), and octahedral (1T), define two distinct structural phases. (1) This structural variety generates important consequences in the materials properties, for example, MoSe2 presents a semiconductor behavior in the 1H configuration, which is the most energetically stable, whereas a metallic behavior occurs for the 1T structure. Therefore, there is a great interest in understanding and controlling the mechanisms of relative stability between these two TMD phases. (3) In this work, we investigated the relative stability of octahedral and trigonal prismatic MoSe2 flakes, ranging from 15 (45) to 192 (576) formula units (atoms), by means of density functional theory calculations. We found that the structure size has an important effect on the relative energy between 1T and 1H structures, and that the 1T phase becomes more stable for small sized flakes. The 1T structure has a preference to adopt a distorted configuration, which can be explained by Peierls transition, and such distortion has an important contribution to increase the stability of this phase. In contrast, the 1H flakes exhibit only significant reconstructions on their edges and lower decreases of energy from reconstructions compared with 1T. Our findings contribute to obtain a deeper understanding of the phase transitions in TMDs.

Palavras-chave: Transition metal dichalcogenides. Two-dimensional materials. Density functional theory.

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