Phase Transition of MoS2 Bilayer Structures - DTU Orbit (10/12/2018)

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In the present study, using density functional calculations we have investigated a possible mechanism for the structural phase transition of the semiconducting bilayer 2H-MoS2 via lithiation. The results indicate that the addition of lithium to the bilayer 2H-MoS2 transforms the bilayer to a heterostructure of the 2H and 1T structures instead of a complete conversion to the 1T bilayer structure. Therefore, we propose that the desired synthesis of the 1T-MoS2 from the bulk 2H-MoS2 takes place through the hybrid 2H-1T structure. Our finding gives physical insight into the experimentally described microscopic mechanism of the phase transition in MoS2 and enriches the atomic scale understanding of the interaction of MoS2 with the alkali ions and other transition metal dichalcogenides manifesting a similar phase transition.

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