Abstract Submitted
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First-principles study of electronic structures and phase transitions of lithiated molybdenum disulphide[1] JUN LI, XIAOBO CHEN, Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences, Ningbo 315201 PR China, NINGBO INSTITUTE OF MATERIAL TECHNOLOGY AND ENGINEERING TEAM — By first-principles calculations, electronic structures of MoS2, intercalation-induced 2H to 1T phase transition and reversibility are investigated. It is revealed that change of interlayer stacking from 2H to 3R imposes negligible influence on the band structure and stability of MoS2. In contrast, the change of intralayer stacking from 2H to 1T changes the character of p-d repulsion, resulting in a semiconductor-to-metal transition. We demonstrate that the Kohn-Sham band energy, rather than the coulomb repulsion energy, plays dominant roles in both the phase stabilization and transition during Li intercalation. It is found that the evolution of 1T phase is crucially determined by chemical hardness, which underlies the cycle irreversibility. Due to the charge-density-wave (CDW) phase, Li extraction is impeded by the enhancement of Li-host binding. It is indicated that the cycle reversibility can be improved by electron-donor doping in MoS2, because the resultant pre-reduction of Mo and S eliminates the electron transfer from Li to host.

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