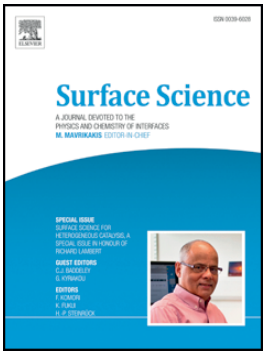


# Interfacial effect on the electrochemical properties of the layered graphene/metal sulfide composites as anode materials for Li-ion batteries

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# Interfacial effect on the electrochemical properties of the layered graphene/metal sulphide composites as anode materials for Li-ion batteries

Yagang Lv, [a] Biao Chen, [a] Naiqin Zhao, [ab] Chunsheng Shi, [a] Chunnian He, [ab] Jiajun Li, [a] and Enzuo Liu[ab*]

[a] School of Materials Science and Engineering and Tianjin Key Laboratory of Composite and Functional Materials, Tianjin University, Tianjin 300072, P.R. China.
[b] Collaborative Innovation Centre of Chemical Science and Engineering, Tianjin 300072, P.R. China.
*Corresponding author. Tel. & Fax. : +86 22 27891371. E-mail address: ezliu@tju.edu.cn (E. Z. Liu).

**ABSTRACT:** The layered graphene/metal sulphide composites exhibit excellent electrochemical properties as anode materials for lithium ion battery, due to the synergistic effect between metal sulfide and graphene which still needs to be further understood. In this study, Li adsorption and diffusion on $MoS_2$ and $SnS_2$ monolayers and $Li_2S$ surface, as well as at their interfaces with graphene, are systematically investigated through first-principles calculations. The analysis of charge density difference, Bader charge, and density of states indicates that the adsorbed Li atoms interact with both the S atoms at metal sulphide surfaces and C atoms in graphene, resulting in larger Li adsorption energies at the interfaces compared with that on the corresponding surfaces, but with almost no enhancement of the energy barriers for Li atom diffusion. The enhanced Li adsorption capability at $Li_2S$/G interface contributes to the extra storage capacity of graphene/metal sulphide composites. Furthermore, the synergistic mechanism between metal sulfide and graphene is revealed. Moreover, band structure analysis shows the electronic conductivity is enhanced with the incorporation of graphene. The results corroborate the interfacial pseudocapacity-like Li atom storage mechanism, and are helpful for the design of layered graphene/metal sulfide composites as anode materials for lithium ion batteries.