Adsorption of Lithium on mirror twin grain boundaries in MoS_2 monolayer

Asghar Ali Jan[1],
Peter Kratzer[1]
[1]*University of Duisburg-Essen, Duisburg, Germany*
asghar.jan@uni-due.de

MoS_2 can be an effective anode material in lithium-ion batteries, as it is scalable at room temperature and has weak van der Waals forces, allowing lithium ions to intercalate between the sheets [1-3]. Additionally, when using MoS_2 as an anode in a lithium-rich environment, the phase transition from the most stable H phase to the T' phase must also be considered [4]. Certain defects, such as sulfur vacancies and grain boundaries, are often present in experimentally synthesized MoS_2 layers [5]. These grain boundaries introduce metallic states within the bulk band gap. As a result, the conductivity of MoS_2 is reduced [6]. Up to now, the H-to-T' phase transition in MoS_2 has been extensively studied, but generally without considering the possible presence of defects such as grain boundaries. Therefore, we have investigated the interaction of lithium intercalation with the grain boundaries present in a MoS_2 monolayer. For example, we examine how the presence of lithium near a mirror twin boundary (MTB) affects the one-dimensional line of charge trapped in the MTB. It is also important to consider the grain boundary formed when a T' phase created from the H phase due to lithium intercalation directly meets the remaining H phase that does not interact with lithium. Our density functional theory calculations provided insights about the stability and electronic properties of these line defects in the presence of lithiation.

References

[1] Zhao L., Wang Y., Wei C., Huang X., Zhang X., Wen G., Particuology, **87** (2024), 240–270.
[2] Samy O., El Moutaouakil A., Energies, **14** (2021), 4586.
[3] Xue J., Xia T., Li T., He J., Wang S., Li W., Ge J., Tan R., Dai Y., He Q., Li N., Zhang G., Duan X., Lin Z., Nature Communications, **16** (2025), 11538.
[4] Wu, Y., Wang, J., Li, Y. et al., Nat. Commun., **13** (2022), 3008 .
[5] Sun, X., Wang, Z. & Fu, Y., Sci Rep, **5** (2015), 18712.
[5] Sobin M. et al., Nano Ex., **6** (2025), 035005.
[6] van der Zande, A., Huang, P., Chenet, D. et al.,Nature Mater., **12** (2013) , 554–561.

Figures

Figure 1: Schematic illustration of Lithium atoms intercalated between bilayer MoS_2, causing phase transition in half of MoS_2. The green, yellow, and purple atoms are Lithium, Suplhur and Molybdenum.