Defect Analysis and Epitaxial Growth of MoS_2 Monolayer Using ReaxFF

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Abstract: The isolation of graphene was a pivotal moment in the discovery of new two-dimensional (2D) materials. Despite its exceptional electronic, optoelectronic, and thermal properties, graphene lacks a band gap, limiting its use in the semiconductor industry. In contrast, transition metal dichalcogenides (TMDs) like MoS_2, which possess a band gap, have emerged as promising semiconductor materials. Consequently, various synthesis techniques have been developed for these materials. In this study, we employ a reactive force field known as "ReaxFF" to explore the atomic-scale mechanisms of vertical MoS_2 growth using a newly proposed method. The results show that Mo-anti sites on MoS_2 single-layer are a necessary step for vertical growth, as they can act as a glue and react with gas phase molecules. Furthermore, our analysis of diffusion of molecules on different defect types in MoS_2 reveals that tri-vacancies are highly reactive, capturing molecules in the gas phase and promoting layer growth.