Computational Study of Process Stability of Non-vdW WS_2/Metal Contact

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Abstract

Defects in layered transition metal dichalcogenides (TMDs), owing to their unavoidable existence after synthesis and processing, play a critical role on many properties and have gain increased attention in the scientific community. In the study, we report on the stability of WS_2 with the removal of single S atom, with the partially-remaining S on one side of W atomic layer, and with the strip of top-layer S atoms, respectively, meant to simulating the defects are introduced during manufacturing process of TMD/metal contacts. Phonon calculations show no imaginary frequency arises due to the symmetry-breaking geometry introduced by the strip of the S atoms on top surface and single O adatom at a S vacancy suggests that the whole system still remains stable by phonon dispersion. Using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code, we propose classical molecular dynamics simulations to reveal that the structural integrity on a relatively large scale of from ~200 to 300 atoms. With top-layer S removal, the freestanding ML WS_2 only demonstrate the wiggle or even warping movement on timescales in the picosecond range, and there is also no sign showing the failure of structural integrity. Our research offers insight into the stability of defective ML TMDs, extremely crucial for the formation of TMD/metal contacts in the next-generation nanoelectronic devices.