**Simulated Scanning Tunneling Microscope Images of Intrinsic Defects in MoTe2**

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Transition metal dichalcogenides (TMDCs) are layered compounds made up of X-TM-X trilayers, where TM and X refer to transition metal and chalcogen atoms, respectively. MoTe2 is one of the representative TMDCs and has been studied extensively due to its high current-on/off ratio implying potential applicability in field-effect transistors [1-5]. In a previous study, intrinsic defects in the single MoTe2 trilayer were investigated systematically and the Te adatom on top of a Te atom was found to be the most stable defect [6]. In this work, we studied intrinsic defects in MoTe2 three trilayers. We performed density functional theory (DFT) calculations by using Vienna *ab-initio* simulation package. We used the PBE exchange-correlation functional in conjunction with the DFT-D3 method to describe the van der Waals (vdW) interaction between the trilayers. We used the 5×5 surface supercell to simulate isolated intrinsic defects. We investigated vacancies, adatoms, interstitials, and vdW gap intercalations for Mo and Te. The most stable structure is found to be the Te adatom on top of a Te atom in both Te-rich and Mo-rich conditions (the corresponding defect formation energies are 1.06 and 1.35 eV) in agreement with the previous study. In addition, we simulated the constant-current STM images for pristine MoTe2 and intrinsic defects within the Tersoff-Hamann approximation. The simulated STM images exhibit strong bias-dependence, which can be used as fingerprints in identifying intrinsic defects.

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