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A first principle study of the naturally aligned bilayer two dimensional (2D) materials DECARLOS TAYLOR, US Army Research Lab - Aberdeen, MAHESH NEUPANE, US Army Rsch Lab - Adelphi, EDWARD BYRD, US Army Research Lab - Aberdeen, SUPENG GE, ROGER LAKE, University of California, Riverside — Semiconducting layered transition metal dichalcogenides (TMDC) exhibit layer stacking and alignment dependent electronic properties resulting from the inter-layer vdW interactions. Independent of the growth conditions, these interactions also contribute to the inter-layer misorientation between the layers during layer-by-layer growth of a multilayer system. Therefore, in order to maintain the commensurability, the size of the supercell must grow exponentially with decreasing misorientation angle and increases from a few atoms for higher angles to several thousand atoms for the smaller angles. This exponential growth in the supercell size limits theoretical study of these systems using first principles methods such as those implemented in VASP and Quantum Espresso. Motivated by these factors, we have conducted a large-scale, first principles study of the electronic properties of the misoriented bilayer 2D materials using the scalable CP2K software package with hybrid basis sets. Using CP2K, the material and device related properties such as band levels, band offsets and work-function as a function of the misorientation angles are calculated and analyzed. The results for the larger misorientation angles with smaller super cell sizes are verified against the results of VASP and Quantum Espresso. A correlation between the misorientation angles, super cell size, and band gaps is established.

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