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A van der Waals density functional study of 1T-Td phase transition in semimetallic bulk MoTe2 and WTe2 HYUN-JUNG KIM, Korea Institute for Advanced Study, IKUTARO HAMADA, National Institute for Materials Science, YOUNG-WOO SON, Korea Institute for Advanced Study, KOREA INSTITUTE FOR ADVANCED STUDY COLLABORATION, NATIONAL INSTITUTE FOR MATERIALS SCIENCE COLLABORATION — Based on the van der Waals density functional (vdW-DF) method, we investigate interlayer interaction and phase stability of orthorhombic (Td) and monoclinic (1T') form of bulk transition metal dichalcogenides (TMD) MoTe2 and WTe2 . We show that a recently proposed revised version of the vdW-DF2 [I. Hamada, Phys. Rev. B 89, 121103(R) (2014)] functional improves the description of the interlayer interaction, thereby computing their most accurate lattice parameters of T_d and 1T' structure successfully as well as electronic properties while several other methods fail to reproduce them. It is also found that the Td structure is energetically favored over the 1T' structure of both MoTe2 and WTe2 . More interestingly, we found that MoTe2 has a transition energy barrier in $T_d \rightarrow$1T' phase transition while WTe2 has no barrier. Such disparate features in transition barrier are consistent with several experimental observations. We will discuss origins of structural phase transition in MoTe2 and its absence in WTe2

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