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van der Waals bonded materials: vanadium pentoxide bulk structure ELISA LONDERO, ELSEBETH SCHROEDER, Chalmers University of Technology — In this work we present a computational study of the layered oxide structure of vanadium pentoxide (V_2O_5) using the vdW-DF functional (M. Dion et al., Phys.Rev.Lett. **92**, 246401 (2004); T. Thonhauser et al., Phys. Rev. B **76**, 125112 (2007); K. Lee et al., Phys. Rev. B **82**, 081101 (2010)) which has proven to be able to capture the essential van der Waals interactions across matter separated by charge voids. We show that these forces play a substantial role for the description of the lattice constants and cohesion of this compound. In addition we document and handle a sensitivity to numerical noise in the evaluation of some exchange versions used with nonlocal correlation.

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