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**A DFT study of metastable *h*-$WO_3$ surfaces** YONGHYUK LEE, TAEHUN LEE, WOOSUN JANG, ALOYSIUS SOON, Department of Materials Science and Engineering, Yonsei University — Polycrystalline $WO_3$ has gained considerable interest as an efficient oxide material for photoreactions [1], and its surface-dependent catalytic properties have been exploited by shape-control crystal engineering of this oxide for photochemistry reactions e.g. water-splitting. Recently, hexagonal single crystal $WO_3$ nanorods with dominant (0001) and $(11\bar{2}0)$ facets were synthesized and these nanorods are found to be highly effective photoanode [2] However, the precise local atomic structures and surface orientations of this metastable *h*-$WO_3$, which are important for understanding surface-dependent photoreactions, are not well studied. In this work, using first-principles density-functional theory (DFT), we consider the various orientations and terminations of *h*-$WO_3$ surfaces and address the predicted nanomorphologies under corresponding experimental conditions based on the DFT-derived Gibbs-Wulff polyhedrons. We provide a microscopic perspective for its potential applications in photoreactions by studying the surface energetics and electronic structure. [1] Y. Ping and G. Galli, *J. Phys. Chem. C* **118**, 6019 (2014); [2] P. M. Rao *et al.*, *Nano Lett.* **14**, 1099 (2014)

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