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vdW-DF $+U$ description of solid oxygen at low pressure SHUSUKE KASAMATSU, TAKEO KATO, OSAMU SUGINO, The Institute for Solid State Physics, the University of Tokyo — Oxygen is known to solidify at low temperature into the paramagnetic cubic γ phase under 54 K, rhombohedral frustrated magnet β phase under 44 K, and the monoclinic antiferromagnetic α phase under 24 K [1]. The structures of these phases result from a subtle balance of the van der Waals and spin-spin interactions between O_2 molecules, and their description using conventional semilocal density functional approximations have proved to be quite unsatisfactory. Recently developed vdW-DF functionals solve the problem partially, but due to inaccruate description of the exchange interaction, the predicted lattice parameters of the α phase are still off by as large as 15% compared to experiment [1]. Semiempirical tuning of spin-spin interaction in the vdW-DF energy functional (vdW-DF-SGC [1]) have also yielded sub-par results. In this work, we report that the DFT+U approach used in combination with certain vdW-DF functionals performs surprisingly well in this regard [2]. This is explained by the correction of overbinding between antiferromagnetic O_2 pairs due to the on-site U interaction applied on the O p orbitals. [1] M. Obata et al.: Phys. Procedia 75, 771 (2015). [2] S. Kasamatsu, T. Kato, and O. Sugino, arXiv:1606.08568 [cond-mat.mtrl-sci]

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