The failure of DFT and DFT+U on predictions of structural and magnetic properties of epsilon-oxygen

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We systematically calculated the structural, magnetic and electronic properties of the epsilon phase of solid oxygen using conventional DFT and DFT+U. While DFT+U can predict the structural epsilon-zeta transition at 80 GPa, which was found at 96 GPa by experiment, conventional DFT calculation only predicts the transition at 50 GPa. On the other hand, conventional DFT shows no magnetic configuration at all pressure above 10 GPa which is consistent with neutron diffraction measurement. The DFT+U predicts the existence of anti-ferromagnetic configuration of the epsilon phase. This talk will discuss the failure of both DFT and DFT+U in comparison with experiments and possible explanations.

Keywords: DFT, DFT+U, solid oxygen, epsilon phase

