Supporting Information for:

Antiferromagnetic vs. non-magnetic $\varepsilon$ phase of solid oxygen. Periodic Density Functional Theory studies using localized atomic basis and the role of exact exchange.

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**Supplementary Material**

The following figures show the pressure evolution of the intramolecular angle in the unit cell for the antiferromagnetic (AF1, AF2) and non-magnetic (NM) unit cell models. Note that this angle remains ca. 90° for the completely non-magnetic structure at all pressures in good agreement with the experimental $C2/m$ crystal group for the $\epsilon$ phase of solid oxygen.

![Intramolecular angle graph](image)

**Fig. S1** Intramolecular angle in the $(O_2)_4$ unit cell for the AF1 (red up triangles), AF2 (red down triangles) and non-magnetic (black squares) models for the $\epsilon$ phase at the PBE level of theory. The experimental value is 90°.
**Fig. S2** Intramolecular angle in the \((O_2)_4\) unit cell for the AF1 (red up triangles), AF2 (red down triangles) and non-magnetic (black squares) models for the \(\varepsilon\) phase at the B3LYP level of theory. The experimental value is 90°.
Fig. S3 Intramolecular angle in the \((O_2)_4\) unit cell for the AF1 (red up triangles), AF2 (red down triangles) and non-magnetic models (black squares) for the \(\varepsilon\) phase at the PBE0 level of theory. The experimental value is 90°.