Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information for:

## Antiferromagnetic vs. non-magnetic ε 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. 90º for the completely non-magnetic structure at all pressures in good agreement with the experimental *C2/m* crystal group for the ε phase of solid oxygen.

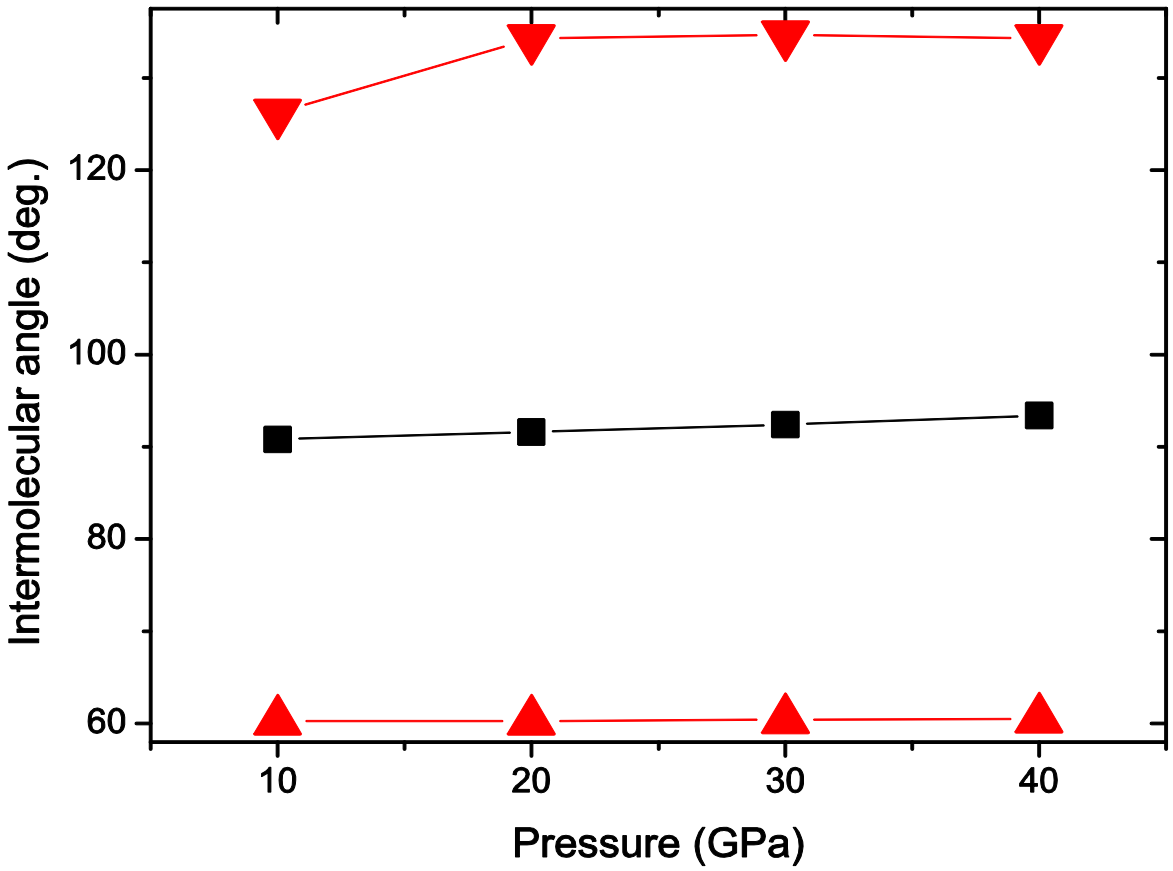


**Fig. S1** Intramolecular angle in the $(O_2)_4$ unit cell for the AF1(red up triangles), AF2 (red down triangles) and non-magnetic (black squares) models for the ε phase at the PBE level of theory. The experimental value is 90º.

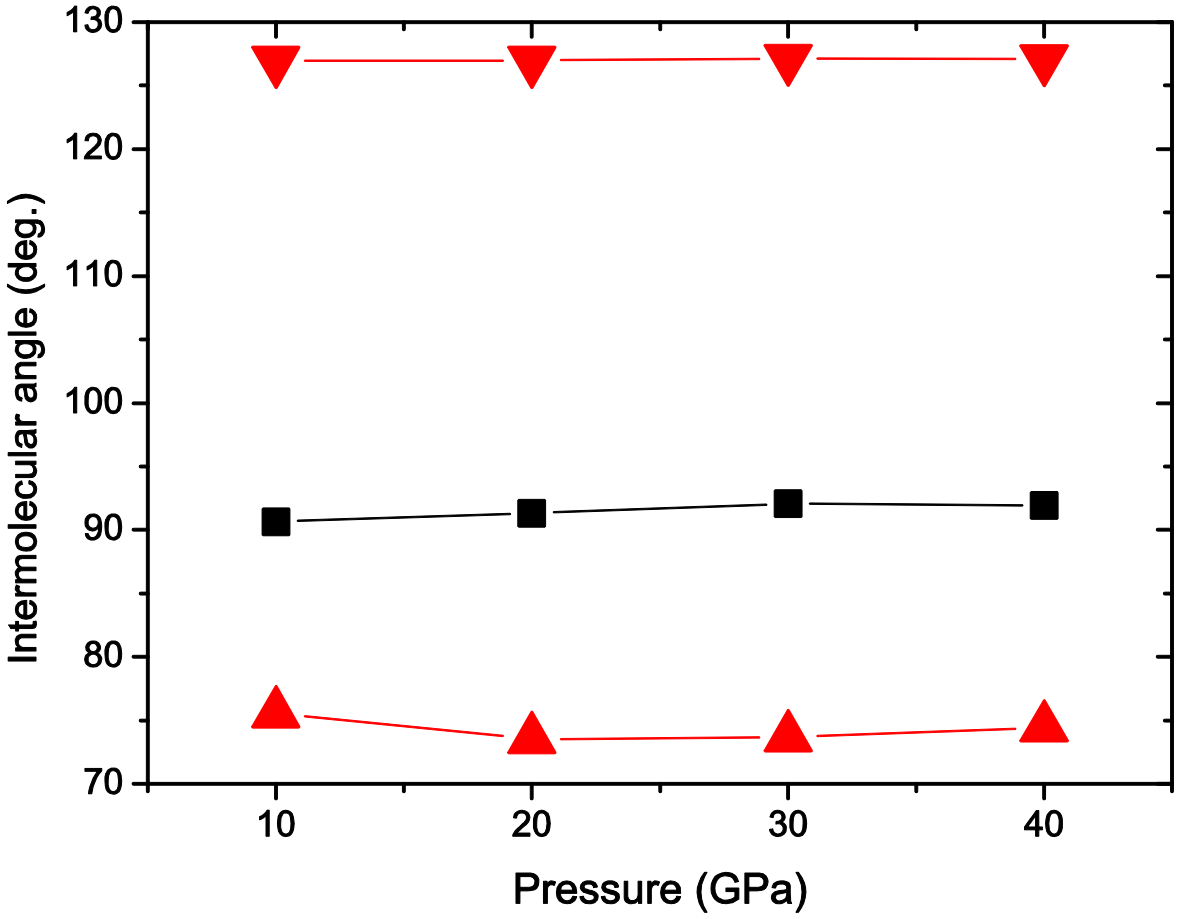


**Fig. S2** Intramolecular angle in the $(O_2)_4$ unit cell for the AF1(red up triangles), AF2 (red down triangles) and non-magnetic (black squares) models for the ε phase at the B3LYP level of theory. The experimental value is 90°.

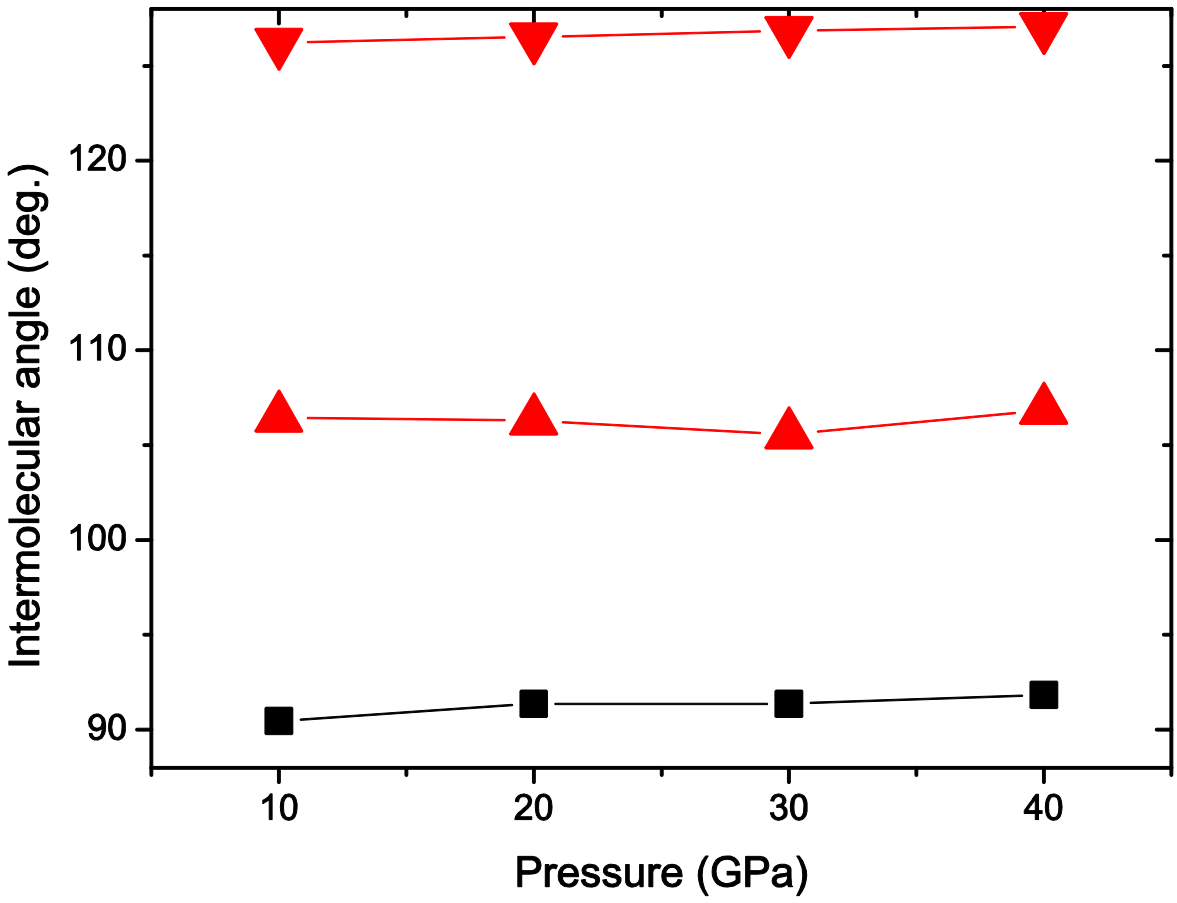


**Fig. S3** Intramolecular angle in the $(O_2)_4$ unit cell for the AF1(red up triangles), AF2 (red down triangles) and non-magnetic models (black squares) for the ε phase at the PBE0 level of theory. The experimental value is 90°.