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Magnetism and vibrations in the phase ϵ of Oxygen TUAN ANH PHAM, University of California, Davis, RALPH GEBAUER, SANDRO SCANDOLO, The Abdus Salam International Centre for Theoretical Physics — Sandwiched between a set of magnetic phases at lower pressure, and a non magnetic phase at higher pressure, the magnetic state of phase ϵ of oxygen has so far been elusive, together with its crystal structure. Neutron diffraction data indicate absence of antiferromagnetism, but do not exclude a ferromagnetic order. The recent refinement of the internal atomic positions from single-crystal diffraction finally provides us with a correct structural model to study the possible occurrence of a magnetic ground state. By employing non-collinear spin-polarized density-functional theory we show that the ground state of ϵ-O_2 is non magnetic. We also calculate vibrational spectra and show that ϵ-O_2 possesses an additional vibron mode with large Raman cross section, not seen in experiments yet.

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