Theoretical studies of the epsilon and dzeta high pressure phases of solid oxygen. Electronic properties, relative stability, finite temperature effects and the transition to the superconducting dzeta phase

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The pressure evolution of the structural and electronic properties of the epsilon and dzeta phases of solid oxygen between10 and 160 GPa are presented utilizing GGA and hybrid DFT descriptions. The role of exact exchange partially present in hybrid functionals is shown to be crucial to explain the relative stability of these phases vs. Pressure. Phononic calculations using hybrid functionals reveal that the ZPE and entropic finite temperature contributions to the Gibbs free enegy are crucial to correctly predict the experimentally observed epsilon -> dzeta phase transition at 110 GPa@300 K.