

Abstract Submitted
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The ε - η' transition in solid oxygen at high pressure¹ SABRI ELATRESH², VAHID ASKARPOUR³, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada, STANIMIR BONEV⁴, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada & Lawrence Livermore National Laboratory, Livermore, California 94550, USA — Despite extensive theoretical and experimental studies, the stability of solid oxygen at high pressure remains an open question. The exact structure of ε -O was only recently defined experimentally as consisting of O₈ units. More recent measurements have indicated that a new phase, η' -O, may be stable above ε -O in the pressure range from 44 to 90 GPa and at temperatures near 1000 K. However, the supporting experimental evidence is not conclusive. In this work, we study the phase diagram of solid oxygen up to 120 GPa and 1200 K from first principles. Full free energy calculations with hybrid exchange functionals have been performed to establish the mechanical and thermodynamic stability of η' -O. This structure has unusual dynamical properties, which will be discussed. Analysis of the low-temperature stability of ε -O to resolves inconsistencies between previous experimental and theoretical results will be presented as well.

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