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Equation of state of crystalline FeO from diffusion Monte Carlo simulations JINDRICH KOLORENC, LUBOS MITAS, North Carolina State University, Raleigh — We investigate equation of state of stoichiometric FeO (at $T = 0$ K) by means of the diffusion quantum Monte Carlo method (DMC). We find a pressure induced transition from the B1 (rocksalt) structure, which represents the ambient pressure ground state, to the inverse B8 (NiAs) lattice. Experimental evidence for such a transition is still rather controversial, being detected in some measurements and not seen in others. Our DMC estimate for transition pressure, $P = 65 \pm 5$ GPa, is compared to outcome of other computational approaches, such as the density functional theory combined with hybrid exchange-correlation functionals.

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