# Diffusion Monte Carlo study of compressed FeO

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We investigate equation of state of stoichiometric FeO (at $T = 0\,\mathrm{K}$) by means of the fixed-node diffusion Monte Carlo method (FN-DMC). We evaluate the critical pressure of structural phase transition from the B1 (rocksalt-type) structure, which represents the ambient pressure ground state, to the inverse B8 (NiAs-type) lattice. In our simulations, fermionic nodes are fixed to those of a Slater determinant constructed of one-particle orbitals that are provided by Kohn–Sham equations with a hybrid density functional. Dependence of the FN-DMC total energy on the exact-exchange proportion in the employed functional is discussed.

[1] J. Kolorenč and L. Mitas, arXiv:0712.3610