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Quantum Monte Carlo Study on NiO crystal RYO MAEZONO[1], National Institute for Materials Science, M.D. TOWLER, TCM Group, Cavendish Laboratory, University of Cambridge, R.J. NEEDS, TCM Group, Cavendish Laboratory, University of Cambridge — Quantum Monte Carlo (QMC) calculations using the variational (VMC) and diffusion (DMC) methods is performed on NiO crystal with gaussian basis and pseudo potentials. We report calculations of energy-volume plots obtained by VMC and DMC with 2*2*2 (16 ions) and 4*4*4 (128 ions) simulation cells. In order to obtain smooth dependences careful optimizations of the basis set at each lattice constant turned out to be indispensable, as well as the larger (4*4*4) simulation cell. The cohesive energy obtained by VMC (without Jastrow function) is around 6.6 eV, while DMC gives around 9.3 eV (near to the experimental value as 9.5 eV, though the present QMC is assuming ferromagnetic ordering).

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