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Quantum Monte Carlo calculations of NiO RYO MAEZONO, Japan Advanced Institute of Science and Technology, Japan., MIKE D. TOWLER, RICHARD. J. NEEDS, TCM, Cavendish Laboratory, University of Cambridge, U.K. — We describe variational and diffusion quantum Monte Carlo (VMC and DMC) calculations [1] of NiO using a 1024-electron simulation cell. We have used a smooth, norm-conserving, Dirac-Fock pseudopotential [2] in our work. Our trial wave functions were of Slater-Jastrow form, containing orbitals generated in Gaussian-basis UHF periodic calculations. Jastrow factor is optimized using variance minimization with optimized cutoff lengths using the same scheme as our previous work. [4] We apply the lattice regulated scheme [5] to evaluate non-local pseudopotentials in DMC and find the scheme improves the smoothness of the energy-volume curve.

[1] CASINO ver.2.1 User Manual, University of Cambridge (2007).
[2] J.R. Trail *et.al.*, J. Chem. Phys. **122**, 014112 (2005).
[3] CRYSTAL98 User's Manual, University of Torino (1998).
[4] Ryo Maezono *et.al.*, Phys. Rev. Lett., **98**, 025701 (2007).
[5] Michele Casula, Phys. Rev. B **74**, 161102R (2006).

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