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The equation of state of diamond from quantum Monte Carlo calculations RYO MAEZONO[1], National Institute for Materials Science, Japan., ANDREA MA, TCM, Cavendish Laboratory, University of Cambrigde, U.K., MIKE D. TOWLER, TCM, Cavendish Laboratory, University of Cambrigde, U.K., NEIL D. DRUMMOND, TCM, Cavendish Laboratory, University of Cambrigde, U.K., RICHARD J. NEEDS, TCM, Cavendish Laboratory, University of Cambrigde, U.K. — We describe variational and diffusion quantum Monte Carlo (VMC and DMC) calculations that have been performed to evaluate the elastic properties of diamond up to pressures of about 500 GPa. We have used a smooth, norm-conserving, Hartree-Fock carbon pseudopotential in our work. Our trial wave functions were of Slater-Jastrow form, containing orbitals generated in plane-wave DFT-GGA calculations, which were re-expanded in a blip-function basis set. We propose a new scheme for determining the cutoff lengths that occur in our Jastrow factor. Using a 512-electron simulation cell, and fitting a Vinet equation of state to our energy-volume data, we have calculated the equilibrium lattice constant (A, in Angstrom), bulk modulus (B, in GPa), and pressure derivative of the bulk modulus (B') to be (A,B,B')=(3.547, 4.83, 3.43) within VMC and (3.563, 4.52, 3.61) within DMC, as compared with the experimental values of (A,B,B')=(3.567, 4.4-4.5, 3.0-4.0).

[1]PREST, JST, Japan

Ryo Maezono
National Institute for Materials Science, Japan.

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