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Quantum Monte Carlo Study of Surface Energy
CHENG-RONG HSING, CHING-MING WEI, IAMS, Academia Sinica, Taipei 10617, Taiwan — The accuracy of Density Functional Theory (DFT) is based on the exchange-correlation approximation used and needs to be checked by highly accurate quantum many-body approaches. We have performed calculations of the surface energies using the state-of-the-art diffusion quantum Monte Carlo (QMC) method to examine the accuracy of LDA and GGA (PBE) functionals in the study of surface energy. The systems studied include NaCl(100), MgO(100), CaO(100), TiO_2(110), Si(100)-(2x2), C(100)-(2x2), and Ge(100)-(2x2) surfaces. Our results indicate that (i) the surface energy by DMC is always larger than the surface energy by LDA; and (ii) the surface energy by LDA is always larger than the surface energy by GGA. For the surface energies of NaCl(100) and MgO(100), the DMC results reproduce the experimental measured values accurately. To conclude, when compared the surface energies obtained by DFT and DMC, the results predicted by DFT using either LDA or GGA functional are underestimated.

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