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Computations of Surface Energy by Diffusion Quantum Monte Carlo Method[1] CHENG-RONG HSING, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica — One of the most important quantities in studying a surface is the surface energy, but the direct experimental measurement is difficult. Therefore theoretical modelling is very important. Nowadays, density functional theory (DFT) is the most commonly used electronic structure method for studying material properties; however, the accuracy of DFT results often depends on the choice of exchange-correlation (XC) functional. By using a more accurate method for treating XC effects, the diffusion quantum Monte Carlo (DMC) method [Rev. Mod. Phys. 73, 33 (2001)] has been applied to study MgO and LiH surfaces [J. Phys.: Condens. Matter 18, L435L440 (2006); Phys. Rev. B 82, 165431 (2010)]. The DMC results reveal that the local density approximation (LDA) predicts a better value than the generalized gradient approximation (GGA). In this work, we present the results of the surface energy for various surfaces (NaCl, LiH, MgO, TiO2, C, Si, Be, Mg, Al and Al2O3) using DMC and DFT with LDA, PBE and PBEsol functionals. Taking DMC surface energies as the benchmark, LDA, PBE and PBEsol functionals underestimate the surface energy, except for LiH, Be, Mg and Al2O3 surfaces where LDA and PBEsol predict the similar values as DMC calculation.

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