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Quantum Monte Carlo studies for the CO adsorption on late transition metal (111) surfaces[1] CHENG-RONG HSING, Institute of Atomic and Molecular Sciences, Academia Sinica, CHUN-MING CHANG, Department of Physics, National Dong Hwa University, CHING CHENG, Department of Physics, National Cheng Kung University, CHING-MING WEI, Institute of Atomic and Molecular Sciences, Academia Sinica — With the rapid development of computers, Density Functional Theory(DFT) has been extensively used to study the physical and chemical properties of materials. However, the major challenge for DFT approaches is whether the exchange-correlation(XC) functionals can describe the system correctly. It is therefore vital to use the highly accurate Quantum Monte Carlo(QMC) method to examine the accuracy of the presently available XC functionals. In this talk, we will present the DMC(diffusion QMC) results in studying the adsorption of CO on the late transition metal (111) surface. It is well known that the LDA and GGA results predict the preference of FCC site. However, the diffuse-LEED experiment concluded that CO adsorbed on atop(88%) and bridge(12%) site. The current DMC results agree with the experimental findings. In order to investigate the failure of LDA and GGA predictions, the DMC calculations are also performed to study the CO adsorption on other (111) surfaces(Rh, Ir, Cu). It is interesting to observe that GGA predicts similar adsorption energies on the atop site as DMC, but overestimates the adsorption energy for the other adsorption sites(bridge, HCP and FCC). The results explain why GGA tends to favor the higher coordination adsorption sites.

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Cheng-Rong Hsing
Institute of Atomic and Molecular Sciences, Academia Sinica

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