The nonlocal correlation as the solution of the CO puzzle problem
PREDRAG LAZIC, FZ-Juelich, Germany, MOJTABA ALAEI, Isfahan University of Technology, Iran, NICOLAE ATODIRESEI, Osaka University, Japan, VASILE CACIUC, FZ-Juelich, Germany, RADOVAN BRAKO, Rudjer Boskovic Institute, Croatia, STEFAN BLUEGEL, FZ-Juelich, Germany — For the last 20 years the Density Functional Theory (DFT) has been the standard approach for the calculation of chemisorption, adsorption, chemical reactions and electronic structure in general. Despite the great successes of the theory in predicting adsorption energies and other properties for many systems it turns out that the theory fails to predict correctly the adsorption site preference for the CO molecule on (111) surfaces of Pt, Cu and Rh, for example. The DFT calculations predict that the highly coordinated FCC (hollow) site adsorption is preferred over the top site adsorption, while experiments show unambiguously that CO adsorbs into the top site. Also, the calculated adsorption energies do not match well the experimental values. CO molecule chemisorption on these surfaces is a type of system in which one would expect DFT theory in its present implementation with semi-local (GGA) functionals to work well. We show that the inclusion of the nonlocal correlation into the DFT calculations of CO chemisorption through vdW-DF functional largely solves the discrepancies known as the CO puzzle problem.

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