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Ab initio phase diagram of oxygen adsorption on W(110)[1]
MARKUS STÖHR, University of Vienna, Department of Physical Chemistry, STEFAN MÜLLER, University of Erlangen-Nuremberg, Chair of Solid State Physics, RAIMUND PODLOUCKY, University of Vienna, Department of Physical Chemistry — Oxygen adsorption on the tungsten (110) surface has been studied experimentally as well as by semi-empirical theoretical approaches. Up to now, no *ab initio* modelling of this adsorption process has been done, for which we present a combined density functional theory (DFT) and cluster expansion (CE) study. For the CE all lateral unit cells with up to 12 atoms were considered. The (2x1) and (2x2) adsorption phases are found to be ground states which is confirmed experimentally [1]. On the basis of effective cluster interactions Monte Carlo (MC) simulations were performed in order to access finite temperature effects. Concerning the atomic structure we find excellent agreement to experimental scanning tunneling microscopy studies [2]. The temperature and coverage dependent short range order parameter is analyzed. From the results of the applied DFT, CE and MC approaches an *ab inito* surface phase phase diagram can be derived. [1] Wu et al., Physical Review B **39**, 7595 (1989). [2] Johnson et al., Phys. Rev. Lett., **71**, 1055 (1993).

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