The mode of adsorption of water (dissociative versus molecular) as well as its effect on the structural and electronic properties of the FeO₂(001) surface is studied using density functional theory (DFT) calculations with the FP-LAPW method in the WIEN2k implementation. We vary the concentration of water and hydroxyl groups starting from a single water molecule per (√2×√2)R₄5° unit cell and compare the surface stability of the different terminations as a function of the O₂ and H₂O partial pressure within the framework of ab-initio thermodynamics. Over a substantial range above the oxygen and water poor conditions, a clean Jahn-Teller distorted bulk termination is most favorable (modified B-layer) [1]. With increasing water pressure a water monomer, parallel to the surface, is stably fixed on a hydroxylated B-layer is stabilized. The calculations give indications of a lifting of the (√2×√2)R₄5°-reconstruction upon hydroxylation, consistent with low energy electron diffraction (LEED) measurements. [1] R. Pentcheva et al., Phys. Rev. Lett. 94, 126101 (2005).

O 86.2 Fri 9:45 MA 141 Water adosrtion at low-indices (001) and (100) V2O5 surfaces. — PAVEL HEUDUK and MALGORZATA WITKO — Institute of Catalysis and Surface Chemistry, PAS, Krakow, Poland

Vanadia-based materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2]. The VOx materials are well known as the catalysts for numerous number of different chemical processes, as a consequence of an existence of a variety of vacancies at vanadium oxide (VOx) surfaces [2].

In the present study water adsorption at the unsaturated surfaces is examined using cluster DFT approach. In addition a comparison with respect to saturated (010) surface is done. Results of calculations show that water molecule stabilizes at unsaturated surfaces due to the formation of a hydroxyl group. Upon adsorption, with low dissociation energy, it is in contrast to the (010) surface where water molecule undergo stabilization but only due to weak hydrogen bonding and its dissociation does not occur.

O 86.3 Fri 10:00 MA 141 Electronic properties of the active sites present at the (011)MoO2 surface. Periodic and cluster DFT quantum chemical studies — REINATA TONGARZ-SOBIERAJ1, MALGORZATA WITKO1, and ROBERT GRYBOS — 1Institute of Catalysis and Surface Chemistry PAS, Niezapominajek 8, 14-109 Krakow, Poland — 2Faculty of Physics and Center for Computational Materials Science, Universitaet Wien, Sensengasse 8, A-1090 Wien, Austria

DFT method is applied to describe electronic structure of catalytically important (011) surface of molybdenum dioxide. MoO₂ exists in literature mainly as a product of MoO₃ reduction; however the problem of its role in catalytic process is still unsolved. In present paper attention is focused on the properties of surface active sites, both Mo and O, which are present at the selected (011) surface. In addition, comparison of (011)MoO₂ and (100)MoO₃ surfaces is carried out due to a fact that both surfaces contain not only the differently coordinated O sites but also the bare Mo centers. The electronic structure of studied systems is calculated using both periodic (VASP code) and cluster (Stub code) approaches with gradient corrected functional. Local properties of different surfaces sites that are exposed at both surfaces are examined by means of charge densities, bond orders indices and molecular orbital diagrams whereas the global properties of both surfaces are discussed by density of states. The differences (existence of pairs of metallic sites on (011)MoO₂ surface) and similarities (electronic states of bare Mo ions in both surfaces) in electronic properties of active sites are investigated taking adsorption of hydrogen and oxygen as examples.

O 86.4 Fri 10:15 MA 141 Wavefunction-based ab-initio results for the adsorption of CO on Ceria (110) surface — CARSTEN MULLER1, RODRI BERCHEN1, BEATE PAULUS2, and KIRSTI HERMANSSON2, Department of Materials Chemistry, Uppsala University, Lägerhyddsvägen 1, 75121 Uppsala, Sweden — 2Physikalische und Theoretische Chemie, Freie Universität Berlin, Takurstr. 3, 14195 Berlin

For the ab-initio description of the adsorption process on surfaces it is necessary to model all interactions on the same theoretical footing. The standard density functional methods have their difficulties with describing dispersion forces. But especially for the physisorption, where no covalent bonds are formed between the adsorbant and the surface these interactions are essential. They can only well described with wavefunction based correlation methods. With the method of increments [1] it is possible to apply these methods to extended systems. Here we want to present the first application to an adsorption process. As example we have chosen CO on ceria 110 surface. The idea is to partition the correlation part of the adsorption energy according to localized orbital groups of the adsorbant and the individual atoms in the surface. The main part of the binding are the correlation energies of the absorbant with the different atoms of the surface. Therefore, with the method of increments it is not only possible to yield highly accurate results for the adsorption energy, but also gain information about the individual contributions to the adsorption. [1] B. Paulus, Phys. Rep. 428, 1 (2006).
The spatial arrangement of Magnesium Phthalocyanine (MgPc) has been investigated on FeO films grown on Pt(111) with low-temperature STM and STS. The polar oxide film forms a coincidence lattice with the Pt support and exhibits a surface dipole between the Fe(+)/O(-) layers that varies within the Moiré unit cell. The MgPc molecules preferentially adsorb on regions with large dipole strength. The rotational orientation of the molecules, on the other hand, is determined by their interaction with the atomic Fe-O lattice. The influence of the different binding configurations on the electronic structure of MgPc is revealed from spectroscopic investigations.