Apart from its use in photocatalytic and sensing applications, the SrTiO3(001) surface is also receiving increasing attention as a suitable substrate material for thin film growth. For the latter context the numerous reported surface reconstructions, partly in sensitive dependence of the applied annealing temperature, indicate a complex surface kinetics, which needs to be understood and controlled when aiming at growth experiments tailored to the atomic scale. As a first step in this direction we carry out density-functional theory calculations addressing the energetics and electronic properties of adsorbed oxygen atoms at both regular terminations of SrTiO3(001). With the bonding at the SrO-termination in general stronger than at the TiO2-termination, we confirm in both cases the formation of a peroxide ion together with a lattice oxygen atom [1,2]. This gives rise to a non-trivial topology of the potential energy surface for lateral adatom motion, with the most stable adsorption site not corresponding to the one expected from a continuation of the perovskite lattice. The obtained diffusion barriers are about 0.8 eV in the isolated adatom limit, which would suggest that, at least at the studied ideal terminations, oxygen mobility is not a major bottleneck under typical growth conditions. On the other hand, the absolute binding energetics obtained at the level of semi-local and hybrid [1,2] functionals questions a significant presence of such a mobile oxygen adatom species. We therefore extend our discussion to hydrogen and water as a ubiquitous gas phase species and assess a possible stabilization of oxygen adatoms through the formation of surface hydroxyl groups.

Keywords: Strontium titanate; Adsorption; Oxygen; Density Functional Theory

References