Experimental and computational studies of O_2-SnO_2 surface interaction

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Surface properties of solids and the interactions between molecules and solid surfaces are important for many technical reasons. They also involve a range of physical and chemical phenomena of fundamental scientific interest. Therefore, the integration between experimental kinetic methods and theoretical modelling becomes important. The importance of oxygen chemistry at the SnO_2 surface follows from the fact that SnO_2 is used as the active material in gas sensor applications. The operation principle of these sensors is usually based on the measurable conductance response in the bulk material, which is understood in terms of the reactions of the gas molecules with O_2^- and O^- ions adsorbed onto the surface. The role of the lattice oxygen, but in particular, the bridging oxygen atoms on the surface, is also active. Detailed understanding of the reaction mechanisms of various oxygen species at the SnO_2 surface is important, as it offers a way to improve the sensitivity and selectivity of the sensors.

Oxygen adsorption-desorption kinetics at the SnO_2 surface is studied experimentally and computationally. The transient behaviour of various oxygen species is considered. O_2-TPD experiments together with conductance measurements are carried out to create transient kinetic data. The corresponding kinetics is simulated with a kinetic Monte Carlo method.