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Review

The chemistry and physics of zinc oxide surfaces

Christof Wöll *

Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany

Abstract

Metal oxides are virtually everywhere – only gold has the property not to form an oxide on its surface when exposed to the ambient. As a result, understanding the physics and chemistry of oxide surfaces is a topic of pronounced general interest and, of course, also a necessary prerequisite for many technical applications. The most important of these is certainly heterogeneous catalysis, but one has to realize that – under ambient conditions – virtually all phenomena occurring at liquid/metal and gas/metal interfaces are determined by the corresponding oxide. This applies in particular to friction phenomena, adhesion and corrosion. A necessary – but not necessarily sufficient – condition for unravelling the fundamentals governing this complex field is to analyze in some detail elementary chemical and physical processes at oxide surfaces. Although the Surface Science of metal surfaces has seen a major progress in the past decades, for oxides detailed experimental investigations for well-defined single crystal surfaces still represent a formidable challenge – mostly because of technical difficulties (charging), but to some extent also due to fundamental problems related to the stabilization of polar surfaces. As a result, the amount of information available for this class of materials is – compared to that at hand for metals – clearly not satisfactory. A particular disturbing lack of information is that about the presence of hydrogen at oxide surfaces – either as hydroxy-species or in form of metal hydrides.

In the present review we will summarize recent experimental and theoretical information which has become available from single crystal studies on ZnO surfaces. While the number of papers dealing with another oxide, rutile TiO_2, is significantly larger (although titania does not exhibit a polar surface), also for zinc oxide a basis of experimental and theoretical knowledge as been accumulated, which – at least for the non-polar surfaces – allows to understand physico-chemical processes on an atomic level for an increasing number of cases. In particular with regards to the interaction with hydrogen a number of – often surprising – observations have been reported recently. Some of them carry implications for the behaviour of hydrogen on oxide surfaces in general. We will present the

* Tel.: +49 2343225529; fax: +49 2347094182.
E-mail address: woell@pc.ruhr-uni-bochum.de

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