Polarity at complex oxide surfaces and interfaces

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Polar surfaces present an electrostatic instability which requires substantial modifications of the surface charge density in order to be stabilized. Microscopic surface processes related to polarity compensation, such as non-stoichiometric reconstructions, hydroxylation or electronic reconstruction, have been exemplified on various simple oxide surfaces in the last decades and shown to lead to an interesting variety of behaviors [1-3].

While rather scarce for simple oxides, many polar orientations are encountered at mineral surfaces or in more complex oxides and their compensation mechanism may display new features. Relying on first principle simulations and a comparison with experimental data [4], we will discuss polarity at the (100) surface of $NiWO_4$, a compound which belongs to a technologically important family of materials.

Along the same lines, the concept of polarization discontinuity will be applied to the understanding of interfaces between two oxides which are both oriented along a polar direction. Some specificities of polarity compensation in these systems will be highlighted [5].

Finally, from a more technical point of view, we will show that a correct account of polar/non-stoichiometric surface stability may require appropriate first principles methods, beyond simple DFT grandient-corrected approximation, especially when the energetics and electronic characteristics are strongly coupled. The case of the $Cu_2O(111)$ surface will be discussed in this context [6].

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