Ab-initio studies of the (011) and (110) surfaces of rutile VO_2

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Vanadium dioxide is a promising candidate for fast electronic or optical switching. These applications are based on a metal-insulator transition at 340K, where the structure changes from a monoclinic to a rutile phase. Yet this transition is sensitive to the presence of strain or defects, such as oxygen vacancies [1].

In this talk I will present our results on the bulk and surface properties of the VO_2 phases under varying oxygen partial pressure, and compare our results to recent experimental findings. The calculations were performed with the Vienna Ab initio Simulations Package (VASP). We find that standard GGA functionals (PBE) offer an appropriate description of the structural and electronic description of the rutile phase, but more advance functionals such as meta-GGA+U approaches (SCAN) of hybrid functionals have to be employed to capture the electronic properties (such as the band gap of ~0.7 eV) of the monoclinic phases.

In addition, I will discuss the stability of various surface terminations for the rutile (011) and (110) surfaces. We find that the (PBE) surface energy for the bare (110) surface (~20 meV/A^2) is significantly lower than for the (011) surface (~50 meV/A^2). In addition, our results indicate that the (110) surface can be additionally stabilized by a tetrahedral reconstruction under slightly oxidizing conditions.

References:

[1] J. Jeong at el, Science **339**, 1402 (2013).