Ab-initio investigations of the order of K^+ ions on cleaved muscovite mica

Andrea Conti[1], Giada Franceschi[1], Michael Schmid[1], Ulrike Diebold[1], Florian Mittendorfer[1]

[1] *Institute of Applied Physics, Technical University of Vienna (Austria)*

conti@iap.tuwien.ac.at

Model systems based on single crystals can help to provide a better understanding of the chemistry and the catalytic activity of a given oxide surface. Muscovite mica is an interesting material due to its widespread presence in natural environments and its potential use in various technological applications, such as new-generation electronics based on 2D materials, thermal and electrical insulation, and thin-film growth.

In this work, we present DFT calculations on the surface of muscovite mica, a common phyllosilicate whose structure consists of alternating layers of aluminosilicates and K^+ ions. This material easily splits into thin K-terminated sheets, yet the atomistic order of the surface K^+ ions has been, until recently, unknown [1].

Ab-initio calculations using the "Vienna Ab-initio Simulation Package" (VASP) and the metaGGA (r^2SCAN) exchange-correlation functional indicate a close correlation between the distribution of the surface K^+ ions and the arrangement of the subsurface Al^{3+} ions: the K^+ ions preferentially occupy the Al-rich rings. Moreover, the calculated diffusion barriers (between 0.7 and 1 eV) suggest that the K^+ ions are mobile enough at room temperature to occupy the energetically most favorable sites. AFM simulations using the Probe Particle Model [2] are in good agreement with the experimental images.

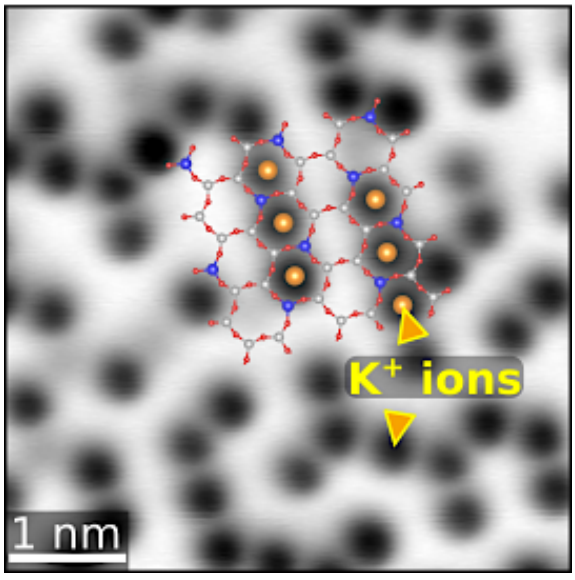

Fig. 1. Constant-height, non-contact AFM image of UHV-cleaved muscovite mica.

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[2] P. Hapala, G. Kichin, C. Wagner, F. S. Tautz, R. Temirov, P. Jelínek, Physical Review B **90**, 085421 (2014)