replacing MAR17-2016-005116

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Polaron-mediated surface reconstruction in the reduced Rutile TiO_2 (110) surface. MICHELE RETICCIOLI, Univ. of Vienna (Austria), MARTIN SETVIN, Vienna Univ. of Technology (Austria), XIANFENG HAO, Yanshan Univ. (China), ULRIKE DIEBOLD, Vienna Univ. of Technology (Austria), CESARE FRANCHINI, Univ. of Vienna (Austria) — The role of polarons is of key importance for the understanding of the fundamental properties and functionalities of TiO_2. We use density functional theory with an on-site Coulomb interaction and molecular dynamics to study the formation and dynamics of small polarons in the reduced rutile (110) surface. We show that excess electrons donated by oxygen-vacancies (V_O) form mobile small polarons that hop easily in subsurface and surface Ti-sites. The polaron formation becomes more favorable by increasing the V_O concentration level (up to 20%) due to the progressively lower energy cost needed to distort the lattice. However, at higher V_O concentration the shortening of the averaged polaron-polaron distance leads to an increased Coulomb repulsion among the trapped charges at the Ti-sites, which weakens this trend. This instability is overtaken by means of a structural 1×2 surface reconstruction, characterized by a distinctively more favorable polaron distribution. The calculations are validated by a direct comparison with experimental AFM and STM data. Our study identifies a fundamentally novel mechanism to drive surface reconstructions and resolves a long standing issue on the origin of the reconstruction in rutile (110) surface.

Michele Reticcioli
University of Vienna (Austria)

Date submitted: 11 Nov 2016 Electronic form version 1.4