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Oxygen storage and release by Ceria: New insights into the mechanism based on STM FRIEDRICH ESCH, CNR-INFM Laboratorio TASC, STEFANO FABRIS, SISSA and CNR-INFM DEMOCRITOS, Trieste, CRISTINA AFRICH, CECILIA BLASETTI, University of Trieste and CNR-INFM Laboratorio TASC, PAOLO FORNASIERO, University of Trieste and INSTM, RENZO ROSEI, GIOVANNI COMELLI, University of Trieste and CNR-INFM Laboratorio TASC
— In the attempt to understand the structure-dependent characteristics of ceria (CeO_2) surfaces with various morphologies (films, nanoparticles, single crystals), we focus on high-resolution scanning tunneling microscopy of a (111) single crystal surface. A new preparation procedure is described that generates one trilayer deep pits on the surface, exposing (001) and (110) steps that can systematically be studied. Pit shapes reflect the surface mobility of ceria and relative stability of the steps. Atomic oxygen exposure leads to the formation of ceria nanoparticles at step edges. Upon reduction, various oxygen vacancies can be distinguished on the (111) terraces and are assigned to single 1st layer vacancies, single 2nd layer vacancies, linear and other vacancy clusters (VCs) by comparison to density functional calculations [1]. It is shown that electron localization determines which VCs can be formed and which can not: VCs expose exclusively reduced Ce^{3+} ions. In linear VCs, that dominate the strongly reduced surface, this occurs by including one single subsurface vacancy per VC. [1] F. Esch et al., Science 309 (2005) 752.

Friedrich Esch
CNR - Lab. TASC-INFM, Trieste

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