
Poster Session | E. Deformation and Fracture Mechanism of Materials

[PO-E2]Poster Session 2

Symposium E

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-37]Ce-terminated (111) surface of CeO_2

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Surface structure and properties of ceria are closely related to the applications of ceria in catalysis. Here, the atomic structures of the (111) surface of CeO_2 nanoparticles have been studied combining aberration-corrected transmission electron microscopy and first-principles calculations. Besides the oxygen termination that have reported extensively previously, the cerium termination has also been revealed by direct atomic imaging, which can be viewed as the simultaneous loss of surface and subsurface oxygen. The stabilization mechanism, electronic structure and magnetism of the surface, and the behavior of oxygen vacancies have been discussed.