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First principle investigation of ZrO_2-CeO_2 heterojunction properties MARCO FRONZI, Materials Nanoarchitectonics Department, National Institute for Material Science, ALESSANDRO DE VITA, Physics Department, King's College London, Strand,London, YOSHITAKA TATEYAMA, ENRICO TRAVERSA, Materials Nanoarchitectonics Department, National Institute for Material Science — Here we present a computational Density Functional Theory approach to analyze the structural and electronic properties of the (100) and (111) ZrO_2-CeO_2 interface. Optimization of the lattice geometry for the separate ZrO_2 and CeO_2 bulks as well as the interface is carried out and the structural morphology is analyzed. The energy formation of the oxygen vacancies are analyzed at different values of lattice parameter, in order to verify its dependency on the strain. Activation energy of the oxygen migration are also calculated in the bulk as well as at the interfaces level. The effect of the doping on the lattice geometry is analyzed for the (111) and (100) interfaces in order to verify its influence on the morphologic disorder.

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