Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO_2(110) Surface

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The dynamics of an *F* center created by an oxygen vacancy on the TiO_2(110) rutile surface has been investigated using *ab initio* molecular dynamics. These simulations uncover a truly complex, time-dependent behavior of fluctuating electron localization topologies in the vicinity of the oxygen vacancy. Although the two excess electrons are found to populate preferentially the second subsurface layer, they occasionally visit surface sites and also the third subsurface layer. This dynamical behavior of the excess charge explains hitherto conflicting interpretations of both theoretical findings and experimental data.

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