

Abstract Submitted  
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**Polarons in rutile TiO<sub>2</sub> surfaces: a non-adiabatic excited-state dynamics study** GRIGORY KOLESOV, School of Engineering and Applied Sciences, Harvard University, DMITRY VINICHENKO, Department of Chemistry and Chemical Biology, Harvard University, GEORGIOS TRITSARIS, School of Engineering and Applied Sciences, Harvard University, CYNTHIA FRIEND, Department of Chemistry and Chemical Biology, Harvard University, EFTHIMIOS KAXIRAS, School of Engineering and Applied Sciences, Department of Physics, Harvard University — Titanium dioxide is one of the most thoroughly studied photocatalytic materials with numerous proposed applications ranging from hydrogen production to cleanup of environmental pollutants. Photocatalytic methoxy splitting on rutile TiO<sub>2</sub> (110) surfaces that leads to formation of formaldehyde has been previously observed in STM and TPD experiments. Due to complexity of such photocatalytic reactions the computational simulations of these reactions are requisite for providing insight into their underlying mechanisms and are crucial for the rational design of the new photocatalysts. Because such simulations are necessarily computationally expensive we developed an efficient methodology based on time-dependent density functional theory (TDDFT) and localized basis set. Our recent non-adiabatic simulations of the photo-catalytic methoxy splitting on titania surface demonstrate an extremely important role played in these reactions by surface and subsurface polarons. Here the polarons serve as electron acceptor sites that participate in driving the reaction and are required to stabilize the reaction products and allow for their subsequent desorption from the surface. In this work we focus on the polarons in rutile titania surfaces and study dynamics of their formation and their properties.

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