

MAR17-2016-020720

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Defects and Small Polarons on Oxide Surfaces¹

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The presence and behavior of defects on the surface of oxides are central in many research areas, including catalysis, photochemistry, solar cells, and surface science in general. Experimental characterization of individual defects and their activities are challenging and often requires special preparations of the surface. First-principles calculations based on density functional theory are a powerful tool to study surfaces and defects, often providing information on properties that are difficult to access experimentally. Here we discuss the behavior of defects on oxide surfaces from the perspective on first-principles calculations. We use the oxygen vacancy on TiO₂ surface as example, a system that has been extensively reported in the literature. Using DFT with a hybrid function, we discuss surface states induced by the defect and localization of the excess charge in the form of small polarons [1,2]. We then discuss the effects of hydrogen and compare the behavior of these defects on the surface with that in the bulk [3]. We also compare our recent results with previous theoretical studies and experiments. Finally, we generalize the findings on TiO₂ to the surfaces of other oxides. [1] M. Setvin, C. Franchini, X. Hao, M. Schmid, A. Janotti, M. Kaltak, C. G. Van de Walle, G. Kresse, and U. Diebold, *Phys. Rev. Lett.* **113**, 086402 (2014). [2] P. G. Moses, , A. Janotti, C. Franchini, G. Kresse, and C. G. Van de Walle, *J. Appl. Phys.* **119**, 181503 (2016). [3] A. Janotti, C. Franchini, J. B. Varley, G. Kresse, and C. G. Van de Walle, *Phys. Status Solidi RRL* **7**, 199 (2013).

¹This work was supported by the NSF.