

Abstract Submitted  
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**DFT calculations of XAS and XPS processes in Ceria cells** B. BARBIELLINI, Northeastern Univ. (NU), T. JARLBORG, U. of Geneva, C. LANE, NU, YUNG JUI WANG, NU and ALS, LBNL, R.S. MARKIEWICZ, NU, LIU ZHI, ZAHID HUSSAIN, ALS, LBNL, A. BANSIL, NU — Final-state effects in X-ray absorption spectroscopy (XAS) and X-ray photoemission(XPS) have been calculated around oxygen vacancies in ceria ( $\text{CeO}_2$ ). The method considers final-state total energies calculated using the constrained density functional theory. In the XAS final state, a core electron is extracted and then added to the valence electrons. The electronic structure is carried out self-consistently under these conditions. After the system has relaxed, one considers the total energy difference between the unperturbed state and the relaxed state to determine the XAS threshold energy. In the XPS final state, one electron is transferred from the ground-state density of states to a homogeneous plane-wave single-particle state. The total energy of the final state is constructed by using an average Kohn-Sham energy corresponding to the hole energy level and the hole density  $\rho_h$ . The present scheme is able to capture important XAS and XPS features observed in experiments when oxygen vacancies are created in ceria. Work supported by the US DOE.

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