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Selective modification of the surface structure of oxide nanoparticles using sub-bandgap photons A. SHLUGER, P. TREVISANUTTO, P. SUSHKO, A. STONEHAM, Department of Physics and Astronomy, University College London, Gower St., London, WC1E 6BT, UK, M. HENYK, K. BECK, A. JOLY, W. HESS, Pacific Northwest National Laboratory, P.O.Box 999, Richland, WA 99352 USA — Controlled manipulation of the physical and chemical properties of nano-structured materials requires correlating their spectroscopic properties and reactivity with specific surface sites. We have demonstrated experimentally that laser excitation of MgO nano-crystalline films and nanocube samples with 4.66 eV photons desorbs neutral O and Mg atoms with hyper-thermal kinetic energies in the range of 0.1–0.4 eV. Using an ab initio embedded cluster approach we developed the mechanisms for the hyper-thermal emission of atomic species. We demonstrate that the desorption of O atoms from 3-coordinated (3C) surface sites occurs via the following steps: i). an exciton is excited at the 3C site; ii) the exciton is ionized, while the remaining electronic hole is trapped at the 3C O site converting it to an O^- radical; iii) absorption of another 4.66 eV photon in the vicinity of the 3C site forms an excited state, which relaxes with desorption of a neutral O atom. Similar process was identified for Mg-terminated 3C site. The proposed general mechanism can be used to control atomic scale modification of insulating surfaces. [1] P.E. Trevisanutto et al., *Surf. Sci.*, **593**, 210 (2005); W.P. Hess et al, *J. Phys. Chem. B*, **109**, 19563 (2005).

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