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O_2 Dissociative Adsorption on Cu_2O(100) with O Vacancies[1] DUY LE, SERGEY STOLBOV, TALAT RAHMAN, University of Central Florida — Cu_2O surfaces and nanoparticles have been shown to have high activity for CO oxidation [1]. As a result of consumption of the surface oxygen during the CO oxidation process on Cu_2O(100), the issue of restoration of the surface composition becomes critical. Through first principles electronic structure calculations of the geometry, activation energy barriers, reaction pathways, and the local densities of electronic states for O_2 dissociative adsorption on the Cu_2O(100) surface with O vacancies, we show that the healing of oxygen vacancies is accompanied by reconstruction of the surface. Our calculations are based on density functional theory in the generalized gradient approximation and usage of ultrasoft pseudopotential method in the plane wave representation. [1] B. White, M. Yin, A. Hall, D. Le, S. Stolbov, T. S. Rahman, N. Turro, and S. O'Brien, *Nano Lett.,* **6**, 2095 (2006).

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