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First-Principles Investigations of Oxygen Vacancies on SnO2 Nanofilms[1] DANIEL CELLUCCI, STEVEN LEWIS, University of Georgia — In recent years multiple critical advances in nanofabrication have allowed for the well-controlled formation of nanocrystals of the n-type semiconductor tin oxide (SnO_2). Because gas sensing in SnO_2 involves changes in surface resistivity as a function of gas concentration, the high surface-to volume ratio of SnO_2 nanocrystals could be leveraged to produce a gas sensor with significantly enhanced sensitivity. A key feature of the sensing mechanism is the facile formation and destruction of oxygen vacancies at (or near) the surface. In this talk I will discuss our ongoing first-principles investigations of surface oxygen vacancies in SnO_2 nanofilms. We have focused on vacancy formation among the so-called bridging oxygen atoms on the (110) surface of rutile SnO_2 as a function of vacancy concentration and film thickness and have studied the effect on local atomic and electronic structure. From a set of first-principles Density Functional Theory calculations on ordered vacancy structures, we have parametrized and tested a lattice-gas model describing vacancy-vacancy interactions. Using this model we have conducted extensive Monte Carlo simulations to investigate the oxygen vacancy phases on SnO_2 (110) as a function of temperature and oxygen vapor pressure.

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