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First-Principles Investigations of Oxygen Vacancies on SnO2 Nanofilms[1] DANIEL CELLUCCI, STEVEN LEWIS, University of Georgia — The n-type semiconductor tin dioxide (SnO2) has long been used as the working material for robust, inexpensive oxidizable-gas sensors. In recent years, advances in nanofabrication have made possible the well-controlled formation of SnO2 nanocrystals. Since gas sensing in SnO2 involves changes in surface resistivity as a function of gas concentration, nanocrystalline SnO2 holds great promise for high-sensitivity gas sensors, due to the high surface-to-volume ratio. 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 SnO2 nanofilms. We have focused on vacancy formation among the so-called bridging oxygen atoms on the (110) surface of rutile SnO2, as a function of vacancy concentration and film thickness, studying the effect on local atomic and electronic structure. This work is the first phase of a longer-term investigation of surface vacancy phases on SnO2 (110) as a function of temperature and oxygen vapor pressure.

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