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Vacancy Ordering and Emergent Electronic Phenomena in $SrTiO_3$ P. GANESH, DILPUNEET S. AIDHY, VALENTINO R. COOPER, PAUL R.C. KENT, Oak Ridge National Laboratory — Electronic complexity in oxides results from the many different types of atomic defects (substitutional, vacancy or interstitial), local strain effects, electrical boundary conditions and other symmetry lowering effects. Among these, oxygen vacancies are one of the most abundant types of defects and can potentially be controlled during oxide growth. We aim to understand what type of oxygen defect configurations form when they are atomically confined to two dimensions in an oxide material i.e. do they prefer to order or prefer disordered configurations, and what types of electronic reconstruction result? Specifically focusing on $SrTiO_3$, one of the constituents of 2DEG forming oxide heterostructures, we have performed extensive density functional theory and cluster expansion based calculations to study vacancy structures and the corresponding changes in the electronic structure. Possibilities for vacancy ordering in the bulk, at surfaces, and at interfaces will be discussed. Acknowledgement: A portion of the research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy. A portion of this research was conducted at the Center for Nanophase Material Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U. S. Department of Energy.

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