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Low Dimensional Oxygen Vacancy Ordering and Diffusion in $SrCrO_{3-\delta}$ PHUONG VU ONG, PETER V. SUSHKO, Physical Computational Sciences Directorate, Pacific Northwest National Laboratory, Richland, WA 99352, U.S.A., PHYSICAL COMPUTATIONAL SCIENCES DIRECTORATE, PACIFIC NORTHWEST NATIONAL LABORATORY, RICHLAND, WA 9 TEAM — Oxygen vacancies (V_O) are known to strongly affect the structure and electronic properties of complex oxides. An ability to control local concentration and spatial distribution of the vacancies, as well as stability and dimensionality of their aggregates, would enable generating novel materials functionalities, such as fast directional charge and mass transport. We use first-principles simulations to study mechanisms of formation, aggregation and diffusion of oxygen vacancies in $SrCrO_{3-\delta}$. We found that at low concentrations oxygen vacancies have a tendency to aggregate into one-dimensional (1D) structures oriented along a [110] direction. These V_O clusters induce rearrangements of oxide ions and conversion of Cr-centered perovskite lattice octahedra into tetrahedra. In turn, aggregation of these 1D V_O clusters enables formation of 2D vacancy aggregates parallel to the (111) plane of the cubic perovskite lattice. We provide a simple physical picture for the formation and growth of such low-dimensional V_O-structures. Moreover, we found mechanisms of V_O migration which enable a diffusion and expansion of the V_O-structures with low activation energies. Our results elucidate the atomic-scale mechanisms of efficient and reversible reduction and oxidation process observed in this material. These mechanisms could be extended to other complex oxides and used in design of high performance electrolytes and cathodes.

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