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Structural and electronic properties of Sr(Zr,Ti)O_3 alloys for use in oxide heterostructures[1] LEIGH WESTON, University of California, Santa Barbara , ANDERSON JANOTTI, University of Delaware, Newark, XIANGYUAN CUI, The University of Sydney, BURAK HIMMETOGLU, University of California, Santa Barbara, CATHERINE STAMPFL, The University of Sydney, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — Sr(Ti,Zr)O_3 alloys are promising materials for use in oxide heterostructures, however the fundamental properties of this system have not yet been characterized. Using hybrid density functional calculations, we study the electronic and structural properties of ordered $SrTi_xZr_{1-x}O_3$ alloys at x=0, 0.25, 0.5, 0.75, and 1. As Ti is added to $SrZrO_3$, the lattice parameter is reduced according to Vegard's law, while the band gap shows a large bowing and is sensitive to the Ti distribution. For x=0.5, arranging the Ti and Zr atoms into a 1×1 $SrZrO_3$/$SrTiO_3$ superlattice along the [001] direction leads to a highly dispersive single band at the conduction-band minimum (CBM) that is absent in the parent compounds, and a direct gap close to that of pure $SrTiO_3$. This is explained by the splitting of the Ti 3d t_{2g} states in the reduced symmetry of the superlattice, lowering the band originating from the Ti 3d_{xy} orbitals. The lifting of the orbital degeneracy around the CBM suppresses scattering due to electron-phonon interactions. We propose that short-period $SrZrO_3$/$SrTiO_3$ superlattices could be exploited to engineer the band structure and improve carrier mobility compared to bulk $SrTiO_3$.

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