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Strain effects on the electron effective mass in $SrTiO_3$[1]

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— Strain can greatly affect the electronic properties of thin layers in epitaxial heterostructures, leading to improved transport properties. In $SrTiO_3$-based heterostructures, strain can lift the degeneracy and modify the order of the states near the conduction-band minimum. Using density functional theory with the screened hybrid functional of Heyd, Scuseria, and Ernzerhof (HSE) we study the effects of strain on the energetic ordering and effective mass of the lowest-energy conduction-band states in $SrTiO_3$3. We predict that biaxial stress in the (001) or (110) planes results in the lowest-energy conduction-band state having significantly smaller electron mass in the in-plane directions compared to unstrained $SrTiO_3$, thus suggesting that pseudomorphic growth is a promising route to increasing the electron mobility in epitaxial films. We propose possible substrates that may lead to $SrTiO_3$ films with enhanced electron mobilities, and report deformation potentials that allow accurate prediction of conduction-band splittings for arbitrary strain configurations.

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