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First-principles study of transport in SrTiO3 BURAK HIMMETOGLU, ANDERSON JANOTTI, HARTWIN PEELAERS, AUDRIUS ALKAUSKAS, CHRIS G VAN DE WALLE, University of California Santa Barbara — As a wide-band-gap semiconductor, SrTiO3 has attracted great interest for electronic device applications. While high electron mobilities of around 30,000 cm2 V-1 s-1 have been observed at low temperatures [1], room temperature mobilities are only on the order of a few cm2 V-1 s-1. These low mobilities pose a significant limitation for electronic device applications. In our work, we investigate the transport properties of n-doped SrTiO3 using first-principles calculations. We compute scattering of electrons with longitudinal optical modes in order to determine the scattering rates for the three conduction bands of SrTiO3. These scattering rates are invoked in Boltzmann transport integrals to calculate room-temperature transport coefficients. Our results indicate the strong impact of longitudinal optical phonon scattering as the main mechanism that leads to small electron mobilities at room temperature. In addition, our analysis provides valuable insights into designing high-mobility and high-thermopower materials, based on band-structure and strain engineering. Work supported by ONR and NSF. [1] J. Son, P. Moetakef, B. Jalan, O. Bierwagen, N. J. Wright, R. Engel-Herbert, and S. Stemmer, Nat. Mater. 9, 482 (2010)

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