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Theory of spin-orbit coupling at LaAlO3/SrTiO3 interfaces and SrTiO3 surfaces ZHICHENG ZHONG, ANNA TOTH, KARSTEN HELD, Vienna University of Technology — A full theoretical understanding of the spin-orbit coupling (SOC) effects at $LaAlO_3/SrTiO_3$ interfaces and $SrTiO_3$ surfaces is still needed. We perform first-principles density-functional-theory calculations and derive from these a simple tight-binding Hamiltonian, through a Wannier function projection and group theoretical analysis. We find striking differences to the standard Rashba theory for spin-orbit coupling in semiconductor heterostructures, because the relevant t_{2g} orbitals are very different from nearly free electrons. The key ingredients to the spin splitting are the atomic SOC and the interface asymmetry, which enters via asymmetric t_{2g} orbital lobes. ArXiv:1209.4705 by Zhicheng Zhong, Anna Toth, Karsten Held

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