Rashba driven superconductivity in incipient ferroelectrics

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SrTiO3 (STO) and KTaO3 (KTO) are known for their proximity to a ferroelectric phase. STO shows bulk superconductivity with a characteristic domelike behavior resembling systems close to a quantum critical point. Several mechanisms have been proposed to link these phenomena, but the abundance of undetermined parameters prevents a definite assessment. We use ab-initio computations supplemented with microscopic modeling to test different coupling models between conduction electrons and the ferroelectric soft transverse mode. In the case of STO, we find that a Rashba-type one-phonon spin-orbit-assisted coupling can explain the magnitude of the critical temperature and the dome-like behavior (Fig. 1). The dome is attributed to a momentum-dependent quenching of the angular momentum due to a competition between spin-orbit and hopping energies. The optimum density for having maximum Tc results in good agreement with experiments without free parameters. These results make the generalized Rashba dynamic coupling to the ferroelectric soft mode a compelling pairing mechanism to understand bulk superconductivity in doped SrTiO3. We will also discuss a two-phonon mechanism and its applicability to these and other materials.

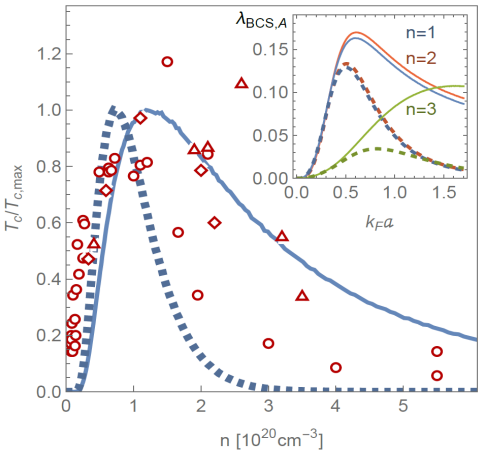

Figure 1. Tc dome (normalized to its maximum value) vs. carrier density. The full (dashed) line neglects (includes) the hardening of the TO mode with density. Inset: band resolved λ_{BCS} using the ab initio results. Open symbols are bulk Tc experimental data from C. S. Koonce et al, PRB 1967 (circles), C. Collignon et al. PRB 2017 (triangles) and Thiemann et al. PRL 2018 (diamonds) using Tc,max = 0.35K.

[1] M.N. Gastiasoro, M.E. Temperini, P. Barone, J. Lorenzana, *Phys. Rev. B*, **2022,** *105,* 224503; arXiv:2210.05753 (PRR in press.)

[2]G. Venditti, M.E. Temperini, P. Barone, J. Lorenzana, M.N. Gastiasoro, J. of Phys.: Materials, **2022,** *6,* 014007.