Doping dependence of the superconducting transition temperature in electron-doped $SrTiO_3$ based on the first-principles calculations

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$SrTiO_3$ is a wide-gap semiconductor with a bandgap of 3.2eV. When *n*-type carriers (electrons) are introduced in $SrTiO_3$ through oxygen reduction[1] or Nb-doping[2], the superconductivity is observed for a wide range of low carrier concentrations $n=10^{18}\sim10^{21}/cm^3$ where the transition temperature T_c shows a characteristic dome shape as a function of n with a peak of $T_c=0.45K$ at $n\sim10^{20}/cm^3$. In addition, a recent experiment for further low carrier concentrations down to $10^{17}/cm^3$ has revealed that T_c shows another dome shape with a peak of $T_c=0.21K$ at $n\sim10^{18}/cm^3$[3] where the number of energy bands across the Fermi level changes from two to one with decreasing n. Theoretically, the T_c dome for $n=10^{18}\sim10^{21}/cm^3$ was well accounted for by the plasmon mechanism of superconductivity with taking into account of the polar optical phonons responsible for the ferroelectric behavior of this system[4]. The details of the energy band dispersions as well as the phonon dispersions, however, have not been explicitly considered there. In the present paper, we investigate the electronic and phonon states of electron-doped $SrTiO_3$ on the basis of the first-principles calculations and discuss the doping dependence of T_c by using the McMillan equation where the effect of the plasmon is included in the effective Coulomb pseudopotential μ^* as recently developed for various doped semiconductors[5,6].

[1] J. F. Schooley *et al*., Phys. Rev. Lett. **14**, 305 (1965).
[2] E. R. Pfeiffera and J. F. Schooley, Phys. Lett. A **29**, 589 (1969).
[2] X. Lin *et al*., Phys. Rev. Lett. **112**, 207002 (2014).
[4] Y. Takada, J. Phys. Soc. Jpn. **49**, 1267 (1980).
[5] K. Sano, M. Seo and K. Nakamura, J. Phys. Soc. Jpn. **88**, 093703 (2019).
[6] K. Sano, Y. Nitta and Y. Ōno, J. Phys. Soc. Jpn. **89**, 113704 (2020).