Ab-initio Insights into the Single Superconducting $CaCuO_2/SrTiO_3$ Interface

Jinjin Cao and Xiaofan Gou*

[1]College of Mechanics and Materials, Hohai University, Nanjing, 211100, China.
*Corresponding Author: Xiaofan Gou. E-mail: xfgou@hhu.edu.cn.

Abstract: In order to achieve higher superconducting transition temperature (T_c), the low dimensional superconducting systems have been the interest in recent years. The recent improved film deposition techniques have allowed the realization of the artificial heterostructures, with atomically flat interfaces. The relatively higher T_c was achieved in these heterosturcture interfaces, which is not present in the single constituent. For instance, the quasi-two-dimensional (quasi-2D) superconductivity was found in the $FeSe/SrTiO_3$ interface with T_c as high as 109 K, which is rather larger than that in the bulk FeSe with T_c of 8 K. Such similar phenomenon also appears in the other quasi-2D system, $CaCuO_2/SrTiO_3$ heterostructure interface with T_c as high as 55 K, where the bulk $CaCuO_2$ is an antiferromagnetic insulator. For the former one $FeSe/SrTiO_3$, lots of reports show that the charge transfer and the interface-enhanced electron-phonon coupling contribute the majority of the enhanced T_c. However, for the latter one $CaCuO_2/SrTiO_3$, only the experiments infer that the charge transfer should be one of the major determining factors, and there is no available theoretical result so far. As the $CaCuO_2/SrTiO_3$ heterostructure can be regarded as another form of cuprate superconductor, then the theoretical investigations should help to forward understanding the mechanism of superconductivity in cuprate and provide an insight into the exploration of new superconductors by interface engineering. Motivated by further uncovering the interface-induced superconductivity in $CaCuO_2/SrTiO_3$, and inspired by the reports on FeSe/SrTiO3, we performed *ab-initio* calculations to study the charge doping effect on the atomic and electronic band structures and electron-phonon interactions in this $CaCuO_2/SrTiO_3$ interface. The microstructure in this interface is identified with the stacking sequence $SrO\text{-}TiO_2\text{-}CaO_x\text{-}CuO_2$, according to the criterion of lowest energy. On the basis of the determined microstructure of interface, the roles of charge transfer and electron-phonon interactions were also identified in determining the interface-induced superconductivity in $CaCuO_2/SrTiO_3$.

Acknowledgements: This work was financially supported by the Fund of the National Science Foundation of China (No. 11672100) and the Fundamental Research Funds for the Central Universities (No. 2018B48714). The authors gratefully acknowledge these financial supports.