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**Understanding the Superconducting Properties of $YBa_2Cu_3O_7$ from First-Principles** GUANG-LIN ZHAO, Southern University and A & M College, Baton Rouge, Louisiana — The observation of high $_{Tc}$ value and an anomalously small isotope effect in $YB_{a2}Cu3O7$ (YBCO) created a great challenge for understanding In order to shed some light on the problem, we integrated the first-principles calculation of electronic structure of the material into the theory of many-body physics for superconductivity and studied the superconducting properties of YBCO. We used two approaches: (1) the generalized Tc equation developed by Abrikosov et al; and (2) the four-dimensional Eliashberg gap equation of strong coupling theory.It is demonstrated from first-principles that the sharp electronic structure around the Fermi level in YBCO, due to extended saddle point singularity, strongly correlate with the anomalous isotope effect in this superconductor. The high Tc value in YBCO around 90 K may mostly be attributed to the high electron density of states (DOS) around Fermi level and high phonon energy in the material. Some experimental evidences including photoemission spectroscopy measurements are also discussed.The work was funded in part by ARO (Award # W911NF-15-1-0483).

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