Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

The Puzzle of Anomalous Isotope Effect in Zr, Nb_3Sn, and $YBa_2Cu_3O_7$ GUANG-LIN ZHAO, Physics Department, Southern University and A&M College — Anomalously small isotope effect in some high and low T_c superconductors such as Zr, Nb_3Sn, $YBa_2Cu_3O_7$ created a great challenge for understanding. To shed light on a clue to solve this puzzle, a new methodology was implemented by integrating first-principles calculations of electronic structures of the materials into the theory of many-body physics for superconductivity. The aim is to seek a unified methodology to calculate the electronic and superconducting properties of these materials. It is shown that the electronic structures of Zr, Nb_3Sn, $YBa_2Cu_3O_7$ are very complex. The electron densities of states around the Fermi level in Zr, Nb_3Sn, $YBa_2Cu_3O_7$ possess sharp variations that could have a significant contribution to the anomalous isotope effect in these superconductors. However, there still exist some differences between the calculated and experimental results that require further research work.

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Date submitted: 01 Nov 2013 Electronic form version 1.4