Superconductivity in noncentrosymmetric $ThCoC_2$ and the effect of Ni doping

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$ThCoC_2$ is a noncentrosymmetric superconductor with $T_c = 2.5$ K, which can be significantly increased by Ni doping to 12 K in $ThCo_{0.6}Ni_{0.4}C_2$. Based on the non-BCS temperature dependence of magnetic penetration depth, superconductivity in $ThCoC_2$ was recently proposed to be a nodal *d*-wave and mediated by the spin fluctuations [1]. Also, non-BCS behaviors of the electronic specific heat and the magnetic upper critical field were reported before. In this work electronic structure, phonons and electron-phonon coupling are studied in $ThCoC_2$ on the basis of ab initio computations. Effect of the spin-orbit coupling on the electronic structure and electron-phonon interaction is analyzed. The thermodynamic properties of the superconducting state are determined numerically by solving Eliashberg equations. The evaluated electron-phonon coupling constant $\lambda = 0.59$ remain in a decent agreement with the experimental estimates, showing that the electron-phonon interaction is strong enough to explain the observed Tc, however it requires an enhanced value of the Coulomb pseudopotential $\mu*$, which may suggest presence of enhanced electronic interactions. Calculated temperature dependence of the electronic specific heat and magnetic penetration depth strongly deviate from the BCS model. Moreover, neither the BCS model nor the presented Eliashberg solutions can explain their experimentally observed temperature dependence, supporting the hypothesis of a non-s-wave gap symmetry in $ThCoC_2$. Finally, effect of Ni doping on electron-phonon coupling is studied using the KKR-CPA method and the strong increase of λ is found, in agreement with experimental results. This further supports the electron-phonon interaction to be the pairing mechanism of superconductivity in this material.

References:

[1] A. Bhattacharyya et al. Phys. Rev. Lett. 122, 147001 (2019).

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