**Electron-Phonon Coupling, Superconductivity and nontrivial Band Topology in NbN Polytypes**

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Materials that show both topological properties and superconductivity received considerable interest because of the realization of Majorana Fermions i.e., particles with their own anti-particles in such condensed matter systems [1]. Therefore, it is highly demanding to investigate for the materials that has topological properties and superconductivity. Niobium Nitride, NbN, a well-known transition metal nitride is a good superconducting material in its cubic structure (δ*-*NbN) with transition temperature Tc of 17.3 K [2]. Recent experiments on hexagonal NbN (ε-NbN) reveal the existence of superconductivity with a Tc of 11.6 K [3]. On the other hand tungsten carbide (WC) type NbN possesses topological properties with band crossing that has three fold degeneracy along a particular k-vector path in the Brillouin zone [4]. Therefore, NbN is a good candidate that show topological properties as well as superconductivity.

Here we study the electronic structure, lattice dynamics and electron-phonon interactions in δ-NbN, ε-NbN and WC-NbN by performing ab initio density functional calculations. The calculated electronic band structures indicate that the Nb *d*-states are dominant near Fermi level (EF). Interestingly, they also reveal that all three NbN polytypes are topological metals. Specifically, δ-NbN and ε -NbN are, respectively, type-II and type-I Dirac metals, while WC-NbN is an emergent topological metal with exotic triply degenerate nodes. The calculated phonon dispersion relations of δ-NbN are in good agreement with neutron scatterring experiments. The phonon density of states and Eliashberg functions show that the electron-phonon coupling in δ-NbN ( λ= 0.98) is much stronger than in ε-NbN (λ= 0.16) and WC-NbN (λ = 0.11). This results in a much higher superconducting transition temperature (Tc = 18 K) than in ε-NbN and WC-NbN (Tc  ≤ 1.0 K). Our findings thus suggest that the three NbN polytypes would provide valuable opportunities for studying exotic phenomena arising from the interplay between superconductivity and band topology.

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