Electronic Structure of $La(Be,N)_2$ with CaB_2C_2-type structure

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Abstract

Layered compounds exhibit attractive physical properties such as superconductivity and magnetism and have garnered considerable interest for their potential in advanced functional materials. Compounds with the CaB_2C_2-type structure are particularly notable. CaB_2C_2 features unique eight-membered rings composed of boron and carbon atoms, which stack along the c-axis with intercalated ions to form its crystal structure. Superconductors such as YB_2C_2 and LuB_2C_2 have been discovered within this structural family [1]. Recent data driven study of related compound suggest that thin-film forms of CaB_2C_2-type and its related compounds may exhibit significantly enhanced superconducting transition temperatures (T_c) [2,3].

In our research, we focus on developing new superconductors by exploring compounds in which the eight-membered rings are composed of elements other than boron and carbon. Specifically, we investigated $La(Be,N)_2$ using first-principles calculations and found that it has the potential to be a superconductor [4]. In $La(Be,N)_2$, the eight-membered rings are formed by beryllium and nitrogen atoms, embedded within a layered crystal framework. Electronic structure calculations indicate that the ground state of $La(Be,N)_2$ is metallic (Fig. 1) and suggest that favorable conditions for superconductivity with calculated maximum $T_c \sim 17$ K.

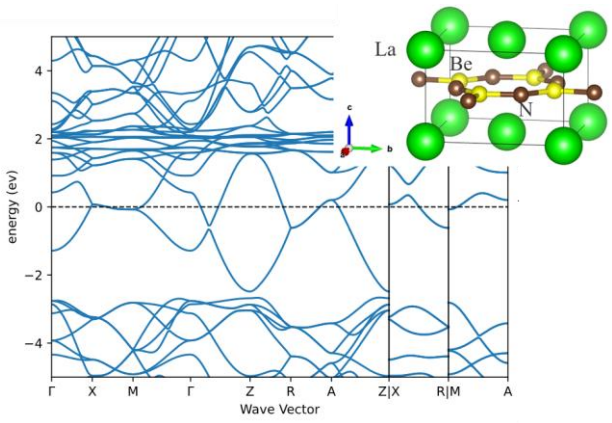

Fig. 1 Band Structure of $La(Be,N)_2$. Inset: crystal structure of $La(Be,N)_2$ (VESTA was used [5]).

References

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Keywaords: First principal calculation, CaB_2C_2-type, Superconductivity