SPIN HALL EFFECT AND SUPERCONDUCTIVITY IN Nb-BASED A15 COMPOUNDS

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INTRODUCTION

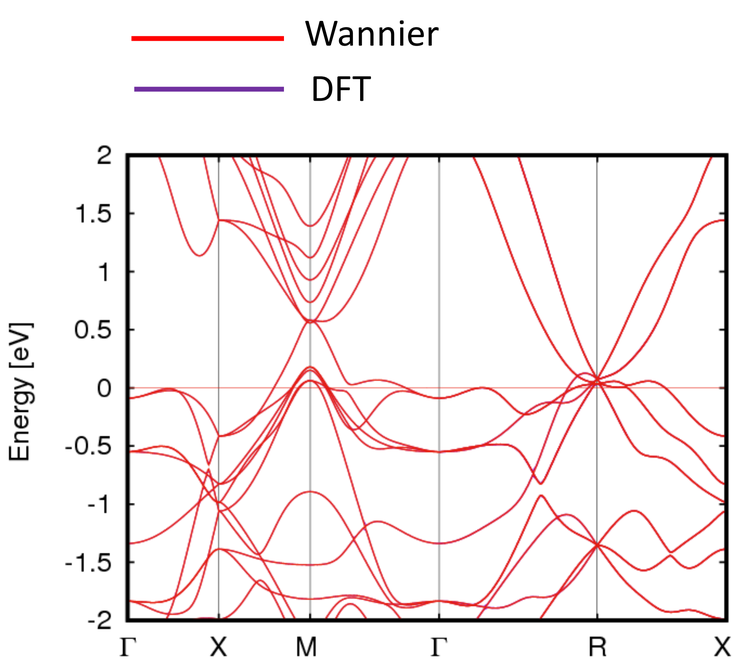
The spin Hall effect (SHE) is the conversion of charge current to spin current and it has become an important topic in recent years due the possible technological applications, like spintronics, creating logic and storage devices based on manipulating both spin and current [1,2]. A large SHE has been predicted in the A15 family of superconductors, due to their bands that present crossings but with the inclusion of spin-orbit coupling (SOC) interaction form hybridization gaps [3].

We are interested in these compounds where the BCS superconductivity can interplay with other spin-orbit effects. We investigate the properties of Nb-based A15 compounds, namely Nb_3Ge, Nb_3Sn and Nb_3Sb by means of ab-initio calculations, Wannier interpolation method and model Hamiltonian.

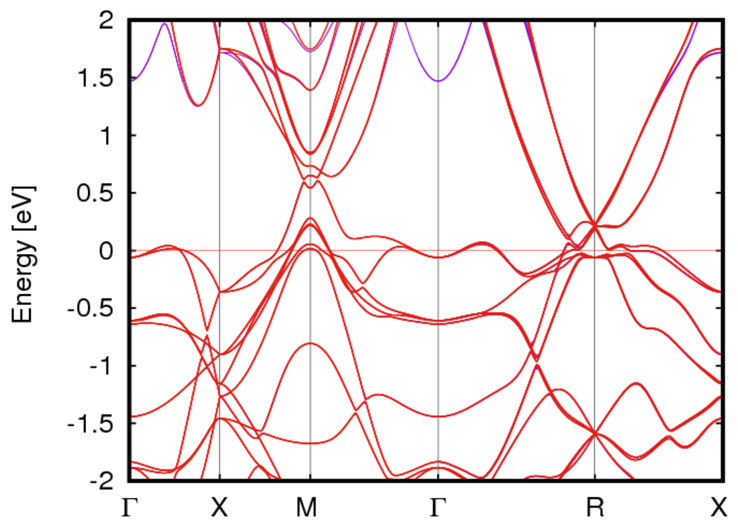
We analyze the band structure and then we extract the tight-binding model through Wannier method and we calculate the spin Hall conductivity (SHC). We get large SHC for Nb_3Ge and lower for Nb_3Sb. This investigation can be performed even in thin films since the DOS of the thin films is reduced by 40% but we still expect large values of T_C and SHC. Then we propose a minimal tight-binding model with t_{2g} Nb-orbitals reproducing the spin-orbit splittings at the R point in this class of compounds. We also calculate the superconding critical temperature in these three Nb-based compounds. We get large values for Nb_3Ge and Nb_3Sn. From our analysis we obtain that Nb_3Ge is the most suitable compound in order to study the interplay between BCS and SHE.

RESULTS

DFT Band structures

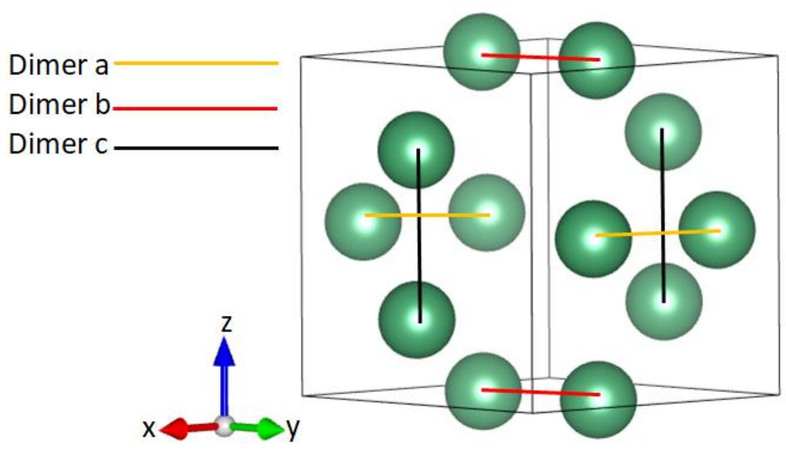


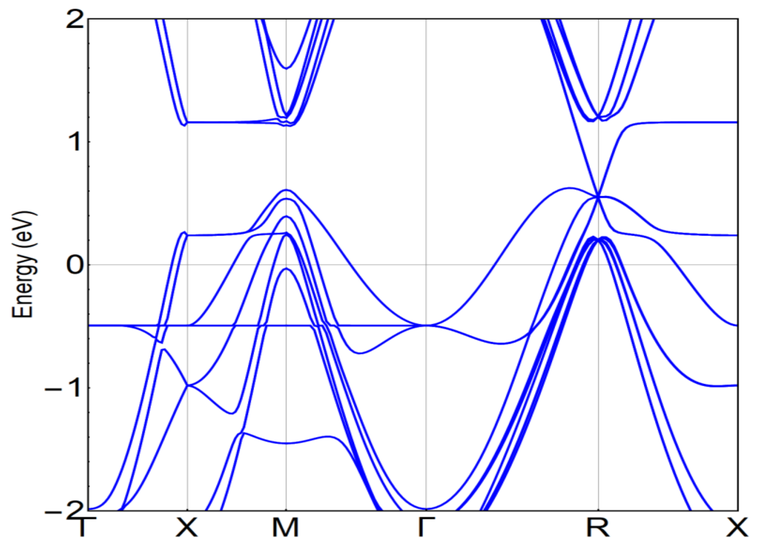
Nb_3Sn, without SOC



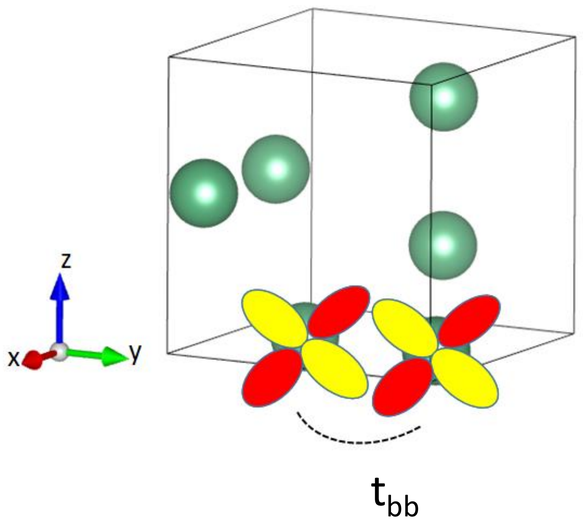
Nb_3Sn, SOC

Minimal tight-binding model

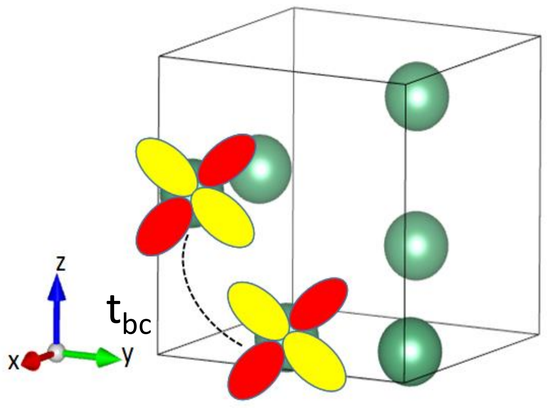




Intra-dimer hopping



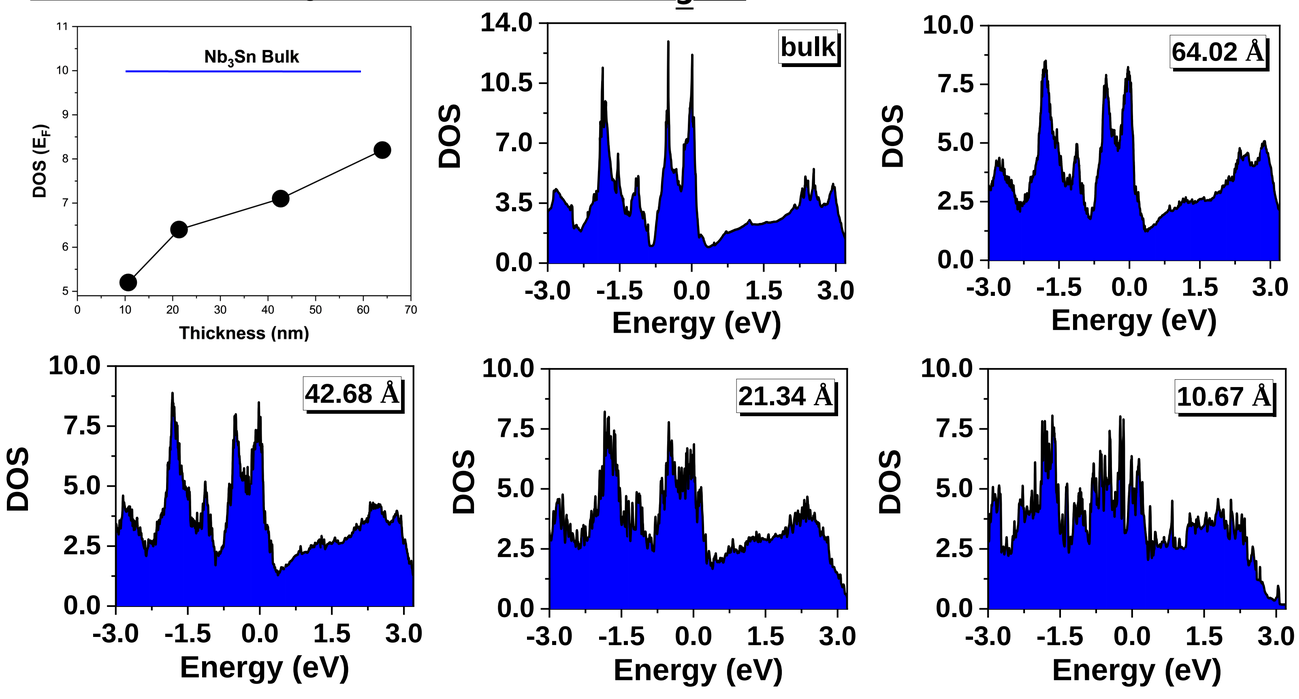
Inter-dimer hopping



$$H = \begin{bmatrix} H_{aa} & H_{ac} & H_{ab} \\ H_{ca} & H_{cc} & H_{cb} \\ H_{ba} & H_{bc} & H_{bb} \end{bmatrix}$$

We produced a tight-binding minimal model for the *d* orbitals of the Nb atoms by considering only the first nearest neighbors Nb-Nb t_{2g} hoppings.

Thickness dependent DOS, Nb_3Sn



Spin Hall conductivities

Compound	Nb_3Sn	Nb_3Ge	Nb_3Sb
SHC [($\hbar$/e)*S/cm]	-983.11	-1691.40	155.29

Superconducting critical temperatures

Compound	Nb_3Sn	Nb_3Ge	Nb_3Sb
T_C [K]	9.9 K	9.6 K	2.3 K

CONCLUSIONS

- We studied Nb-based A15 compounds where the BCS superconductivity can interplay with other spin-orbit effects.
- The Nb-based A15 systems show large SHCs. In particular we get the largest SHC for Nb_3Ge.
- The T_C decreases in the thin films because there is a reduction of the DOS, but we still expect large Tc and large SHC.
- We calculate the superconducting T_C and we get large values around 10 K for Nb_3Ge and Nb_3Sn. In order to study the interplay between BCS and SHE we propose Nb3Ge.

REFERENCES

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