Weyl nodes and chiral edge modes in EuPtSi and $NbSi_2$

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Chiral semimetals, characterized by broken inversion symmetry, host Weyl nodes in both their electronic and phonon band structure. Beyond conventional Weyl nodes, these systems can also support higher-order topological excitations, such as double Weyl nodes with a topological charge of $C = 2$. The resulting chiral edge modes propagate unidirectionally along closed loops surrounding these Weyl nodes, providing clear evidence of their topological properties.

In this study, we investigate the chiral compounds EuPtSi and $NbSi_2$, which crystallize in the $P2_13$ and $P6_222$ space groups, respectively, by analyzing their bulk and slab electronic and phononic properties using first-principles (*ab initio*) calculations. The bulk electronic and phononic band structure of EuPtSi hosts a spin-1 Weyl point at the Γ point and a charge-2 Dirac point at the R point. In contrast, $NbSi_2$ exhibits two Weyl points located at the Γ and K points in the phonon band structure. These topological band crossings give rise to surface states, e.g., electronic and phonon Fermi arcs, that connect nodes with opposite topological charges, resulting in chiral edge modes on the surfaces of both materials. For both compounds, the chiral edge states extend from the center to the boundary of the surface Brillouin zone forming long Fermi arcs. Notably, $NbSi_2$ exhibits a distinct momentum-dependent evolution of its surface phonon arcs, highlighting the rich topological behavior of its phonon spectrum.

Acknowledgments *his work was supported by the National Science Centre (NCN, Poland) under Project No.2021/43/B/ST3/02166 (A.P.).*

References

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