Study of charge density wave, superconductivity and topological in kagome materials

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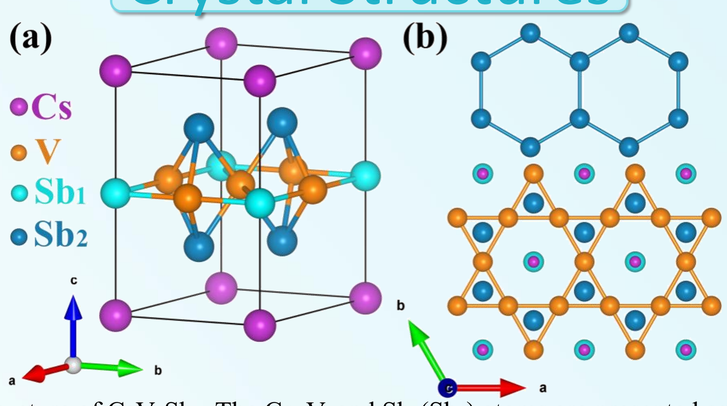
Abstract

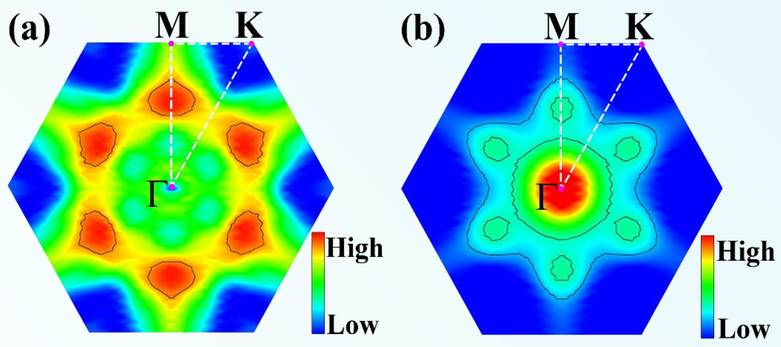
Kagome metals AV_3Sb_5 (A = K, Rb, and Cs) have received intensive research interest due to the presence of charge density waves (CDWs), Z_2 topological surface states, and intriguing pressure-dependent superconductivity (SC). Using first-principles calculations, here we study the origin of the CDW order in CsV_3Sb_5 and its superconducting properties under pressure up to 45 GPa. We reveal that the momentum-dependent electron phonon coupling (EPC) effect plays an important role in the formation of the CDW order. Upon compression, the movement of the van Hove singularity, which induces the change in the density of states at the Fermi level, as well as the redistribution of the EPC, can explain the experimentally observed double superconducting domes. The main contribution to the EPC is varied from in-plane vibrational modes in superconducting area I (2–15 GPa) to out-of-plane modes in superconducting area II (15–45 GPa). Materials prediction through elemental substituting using first-principles calculations is an effective way to guide experimenter to design more interesting materials. To explore more kagome compounds with the coexistence of superconductivity and nontrivial band structure, we predict some AV_3Sb_5-type materials, and then check their stability and investigate their electronic structures, superconductivity. The calculated results (8.02, 5.47, and 3.51 K for $CsTi_3Te_5$, $CsZr_3Te_5$ and $CsHf_3Te_5$, respectively) are clearly higher than those of AV_3Sb_5 family materials. the $CsZr_3Te_5$ and $CsHf_3Te_5$ are also predicted as Z_2 topological metals by calculating the topological invariant and surface states. The coexistence of superconduc_x0002_tivity and nontrivial topological properties in $CsZr_3Te_5$ and $CsHf_3Te_5$ supply guidance for further theoretical and experimental works to seek novel topological superconductors, especially in materials with the AV_3Sb_5-prototype structure.

Crystal Structures

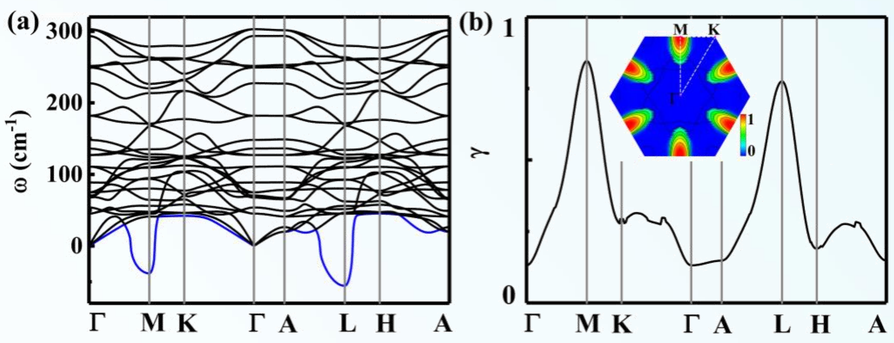


(a) Crystal structure of CsV_3Sb_5. The Cs, V, and Sb_1(Sb_2) atoms are presented as purple, orange, and azure (steel blue) balls, respectively. (b) The graphite net formed by Sb_2 atoms (top) and the two-dimensional kagome lattice formed by V atoms(bottom)

Origin of CDW order in CsV_3Sb_5

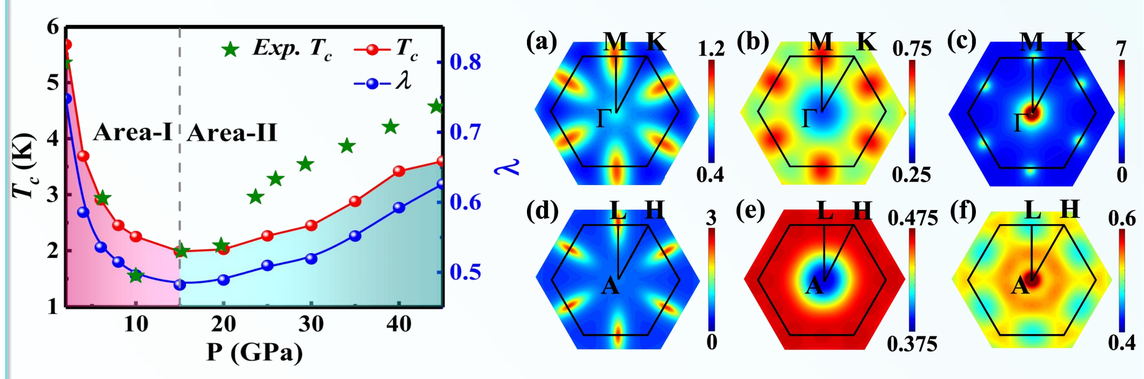


(a) Real and (b) imaginary parts of the electron susceptibility cross section in the plane of $kz = 0$.



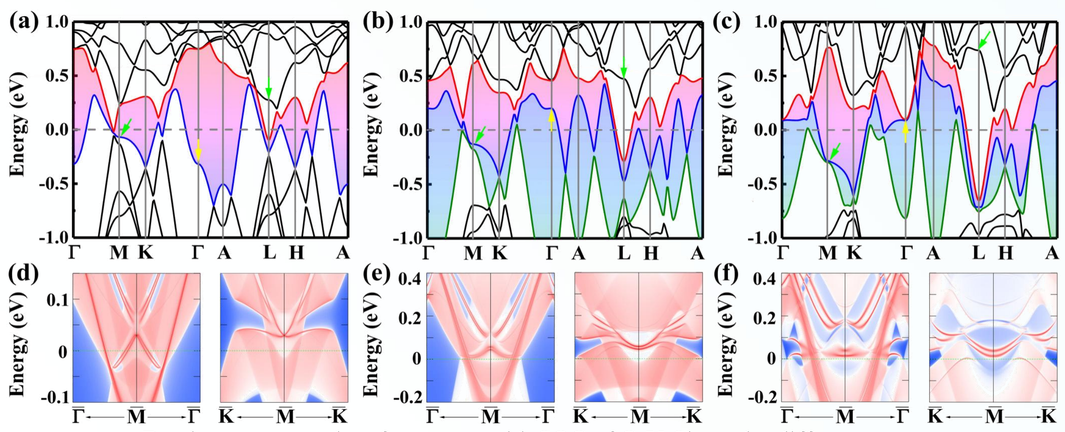
(a) Phonon dispersions and (b) total phonon linewidth of CsV_3Sb_5 under ambient pressure. The inset of (b) is the phonon linewidth γ of the lowest mode in the BZ.

HP controlled SC in CsV_3Sb_5



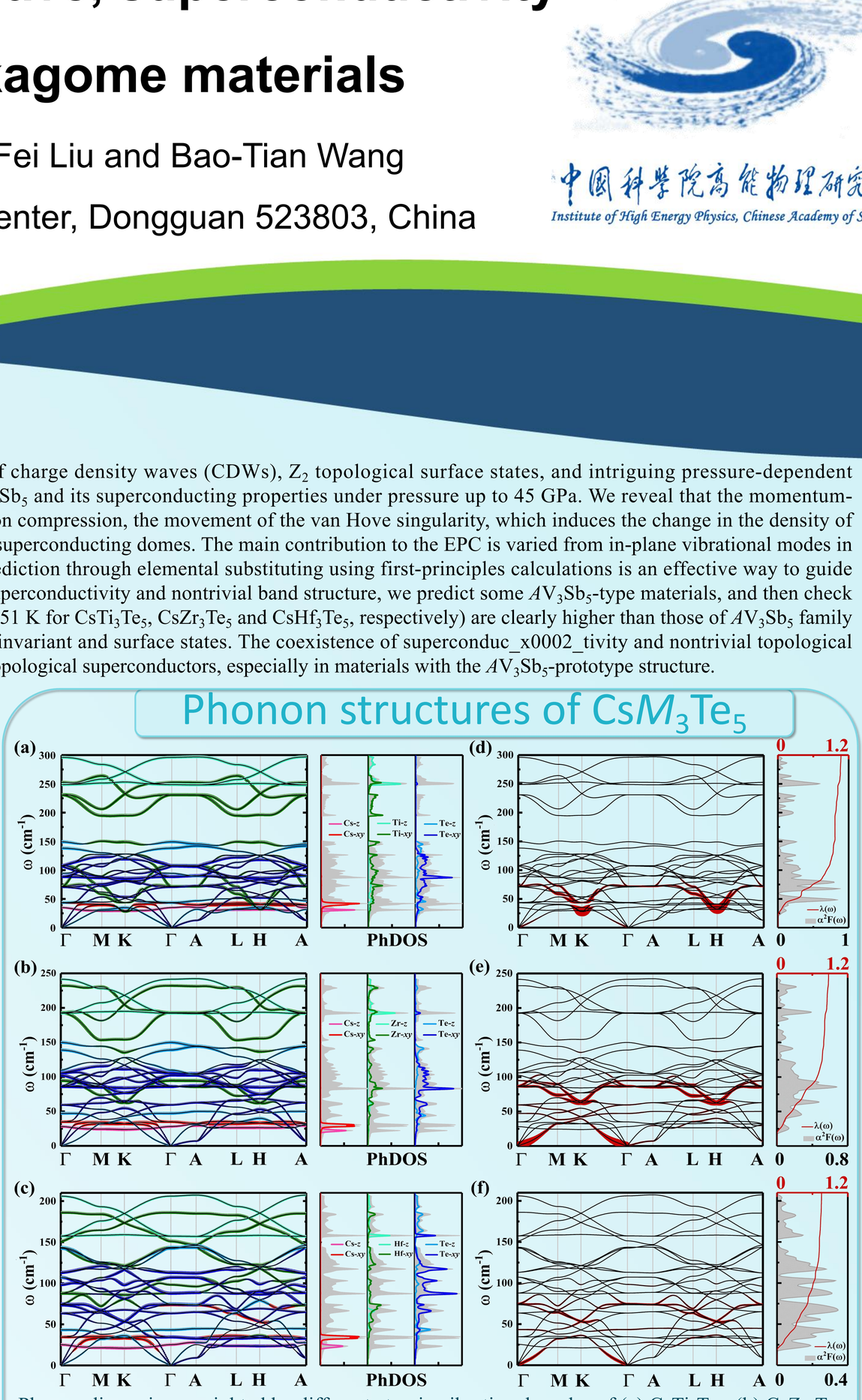
(left panel) The evolutions of T_c (red line) and EPC constant λ (blue line) of CsV_3Sb_5 as functions of pressure. (right panel) The integrated EPC distributions of CsV_3Sb_5 in the plane of qz = 0 under (a) 2, (b) 15, and (c) 45 GPa. The results for the plane $qz = 0.5$ are plotted in (d)–(f), respectively.

topological properties under HP



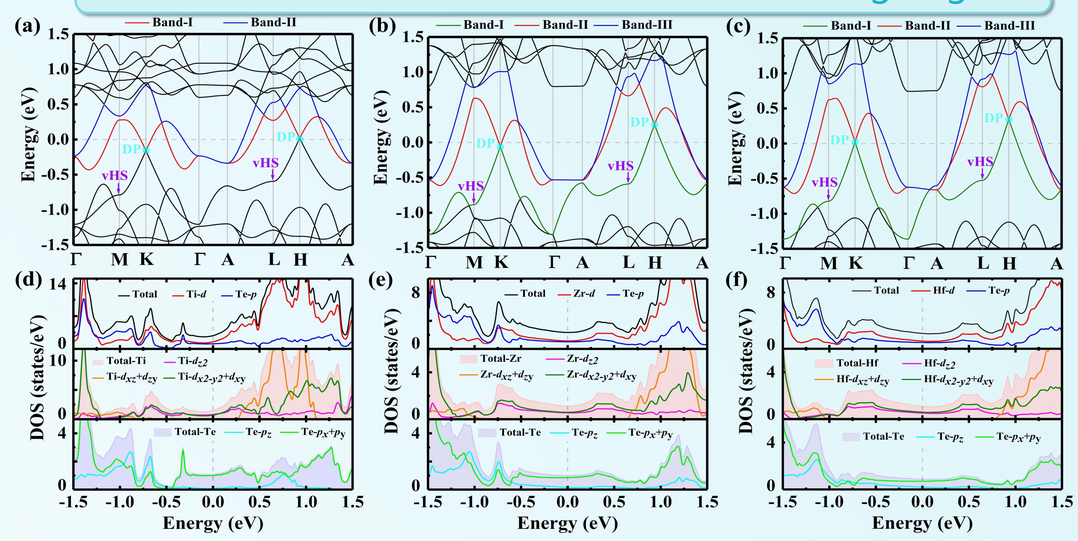
Band structures and surface states with SOC of CsV_3Sb_5 under different pressure.

Phonon structures of CsM_3Te_5



Phonon dispersions weighted by different atomic vibrational modes of (a) $CsTi_3Te_5$, (b) $CsZr_3Te_5$ and (c) $CsHf_3Te_5$. The right panels of (a)-(c) are the total (gray-shaded zone) and vibrational mode-resolved (color lines) PhDOS. Phonon dispersions weighted by the magnitude of the EPC, the Eliashberg spectral function $\alpha^2F(\omega)$, and the integrated strength of EPC $\lambda(\omega)$ for (d) $CsTi_3Te_5$, (e) $CsZr_3Te_5$, and (f) $CsHf_3Te_5$ are also presented.

Electronic structures of CsM_3Te_5



Band structures without SOC effect of (a) $CsTi_3Te_5$, (b) $CsZr_3Te_5$, and (c) $CsHf_3Te_5$. The color lines indicate the bands crossing the Fermi level. The Dirac points and the van Hove singularities are illustrated by the light-blue circles and the purple arrows, respectively. (d) The top panel is the total DOS and the atom-resolved DOSs. The middle and bottom panels are the orbital-resolved DOSs of Ti and Te, respectively. (e) and (f) are same as (d), but for $CsZr_3Te_5$ and $CsHf_3Te_5$, respectively

Conclusion

- The origin of the formation of the CDW order in CsV_3Sb_5 is the momentum-dependent electron phonon coupling (EPC) effect.
- The CsV_3Sb_5 is still a weak BCS superconductor, and the main contribution to the superconductivity is changed from the in-plane modes to the out-of-plane modes with increasing pressure.
- The nontrivial Z_2 nature maintains under pressure up to 45 GPa.
- The CsM_3Te_5 (M=Ti, Zr, Hf) are stable both in thermodynamics and dynamics.
- The superconductivity are evaluated Allen-Dynes-modified McMillan formula, and the T_C (8.02, 5.47, and 3.51 K for $CsTi_3Te_5$, $CsZr_3Te_5$ and $CsHf_3Te_5$, respectively) is higher than the AV_3Sb_5 family materials.
- $CsZr_3Te_5$ and $CsHf_3Te_5$ exhibit nontrivial band structures and could be classified as Z_2 topological metal.

References

[1] **Jian-Guo Si**, Wen-Jian Lu*, Yu-Ping Sun, Peng-Fei Liu, and Bao-Tian Wang*. Charge density wave and pressure-dependent superconductivity in the kagome metal CsV_3Sb_5: A first-principles study.
Phys. Rev. B **105**, 024517 (2022).

[2] **Jian-Guo Si**#, Lan-Ting Shi#, Peng-Fei Liu, Ping Zhang, and Bao-Tian Wang*. Superconductivity and topological properties in kagome metals CsM_3Te_5 (M=Ti, Zr, Hf): A first-principles investigation
Phys. Rev. B **under review**.