Scientists Uncover Clues About the Puzzling Nature of Kagome Metals

Metallic compounds and alloys possess several fascinating properties owing to their peculiar structures and interactions. One of these properties, called charge-density wave (or CDW), is caused by the low-energy excitation of the metal. This CDW order generally occurs due to the interaction between electrons and the collective "wiggling" of the atoms of the metal, termed phonons. The nature of this CDW state has led to extensive research on the phenomenon, and scientists have found certain hallmarks of this state.

One of these hallmarks is the softening or reduction of the frequency of phonons near the transition temperature to the CDW state. Yet, a relatively new class of metal compounds, called Kagome metals, shows no phonon softening near the CDW transition temperature.

To understand this departure from the normal behavior around the CDW state, we studied a simplified two-dimensional CDW state using a phenomenological model. Our model reflects the relationship between variables that one would observe in experiments. By tuning the parameters of the model, like electron interactions and electron-phonon coupling, we were able to induce the CDW state in the model. To reflect the properties of the newly discovered compounds, we also added the probable source of the CDW in these compounds, called the van-Hove-singularity filling, to the model.

We observed that as the temperature reached the CDW transition temperature, a central peak could be observed for a phonon factor. This was accompanied by the hardening of the phonon frequency, as is observed experimentally. This central peak was seen to be associated with the collective density of charges in the metal and the coupling of phonons within.

Our findings provide crucial insight into the possible reasons for the lack of phonon softening in Kagome metals, including the recently discovered AV_3Sb_5 (A = K, Rb, Cs), which demonstrates no phonon softening during the CDW transition.

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