Highlights

RESEARCH AREA 1 - Superconductors and Innovative materials for Energy and Environment - 2022

"Why mercury is a superconductor"

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Despite being the oldest known superconductor, solid mercury is mysteriously absent from all current computational databases of superconductors. The theoretical prediction of its critical temperature (Tc) and full understanding of its unique superconducting behavior remained elusive for over a century. Now, 111 years later, researchers have revisited mercury's properties in a detailed study based on state-of-the-art superconducting density functional theory (DFT).

In fact, mercury is an exception among conventional superconductors, most of which can be accurately described by state-of-the-art DFT calculations. To address mercury's specific challenges, we closely examined all physical properties essential to conventional superconductivity, which is driven by electron-phonon coupling.

Specifically, we included previously overlooked relativistic effects that impact phonon frequencies, refined the treatment of electroncorrelation effects influencing electronic bands, and demonstrated that mercury's *d*-electrons provide an unusual screening effect that enhances superconductivity by reducing Coulomb repulsion among superconducting electrons.

With these refinements, our calculations yielded a prediction for mercury's Tc that is just 2.5% below the observed experimental value. This new understanding on the first-known superconductor not only holds textbook significance but also offers important guidance for future superconductivity research.





