First-principles study of phonon-mediated superconductors

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To explore new superconductors, the key issue is to evaluate the superconducting transition temperatures with sufficient accuracy using high throughput calculations. McMillan's formula has been often used for this purpose and superconductivity in hydrogen sulfide was predicted before the experimental discovery. In the McMillan's formula, however, an empirical parameter is used. Also, the calculation of electron-phonon couplings is time consuming. Thus, more efficient method is required for further exploration of superconductivity. In this talk, first, we show how the Eliashberg study improves the transition temperature of hydrogen sulfide [1]. We calculate all the parameters including Coulomb interaction from first principles and consider the effect of zero-point motion and the phonon anharmonicity. Second, we show an efficient evaluation of electron-phonon couplings [2]. Using this method, we evaluate the transition temperature of $Sn_{1-x}In_xTe_{1-y}Se_y$ and compare the result with the experiment [3]. Application to other materials is also discussed.

References

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