Theoretical Design of Light-Element Superconductors

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Advances in *ab-initio* crystal structure prediction algorithms, methods for calculating electron-phonon interactions, and machine learning have opened the door towards the rational discovery of conventional superconductors with superior behavior. Herein, we report theoretical studies of various light-element based superconductors that are discovered using the XtalOpt evolutionary algorithm [1] for crystal structure prediction, or via high-throughput calculations on prototype structures known to be conducive towards superconductivity. Recent experiments have reported room-temperature superconductivity in SH_3 doped with a third element under pressure. To shed light on the structures that may have been synthesized we carry out a systematic investigation of the effect of doping H_3S by carbon and phosphorus [2, 3], considering different doping schemes. Moreover, we show how a chemical pressure analysis can be useful in designing ternary or quaternary clathrate superhydride superconductors that can be stabilzed to lower pressures.

References

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