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Engineering room-temperature superconductors via ab-initio calculations

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The BCS, or bosonic model of superconductivity, as Little and Ginzburg have argued, can in the case of high-enough frequency of bosonic mode bring in superconductivity at room temperatures. It was further elucidated by Kirzhnits et al., that the condition for existence of the high-temperature superconductivity is closely related with negative values of the real part of dielectric function at finite values of the reciprocal lattice vectors. In view of these findings, the task is to calculate the dielectric function for real materials. Then the poles of this function will indicate existence of bosonic excitations which can serve as a "glue"for Cooper pairing, and if the frequency is high enough, and the dielectric matrix is simultaneously negative this material is a good candidate for very high-Tc superconductivity. Thus, our approach is to elaborate a methodology of ab-initio calculation of the dielectric function of various materials, and then point out appropriate candidates. We used the powerful codes (TDDF with the DP package, used in conjunction with ABINIT) for computing dielectric responses at finite values of the wave vectors in the reciprocal lattice space. Though our report is concerned with the particular problem of superconductivity, the application range of the data processing methodology is much wider. The ability to compute dielectric function of existing and still non-existing (-though being predicted!) materials will have many more repercussions not only in fundamental sciences but also in technology and industry.

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