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Anisotropic Eliashberg Theory of MgB_2

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The superconductivity in magnesium diboride is remarkable, not only for the high transition temperature of 39 K, but also for the anomalous behavior of the superconducting energy gap. We study the electronic structures, phonon structures, and electron-phonon interaction in MgB_2 using the *ab-initio* pseudopotential density functional method. We then construct fully anisotropic Eliashberg equations with momentum-dependent electron-phonon interaction and calculate superconducting properties of MgB_2. Our approach describes the superconducting transition temperature and the isotope effect of the material successfully, and predicts that the superconducting energy gap is nodeless but its value varies strongly on difference pieces of the Fermi surface. The predicted gap values Delta(k) cluster into two groups at low temperature, a small value of ~2 meV and a large one of ~7 meV. This gap structure produces two thresholds in the quasiparticle density of states and increases the specific heat at low temperature due to quasiparticle excitations over the small gap. We have further applied our framework to the cases that MgB_2 is compressed with high pressure, is doped with either electrons or holes, and contains significant amount of impurities. The obtained effects of pressure, doping, and impurities on the superconducting properties including the transition temperature and the superconducting energy gap will be discussed.

References: H. J. Choi, D. Roundy, H. Sun, M. L. Cohen, and S. G. Louie, Nature 418, 758-760 (2002); Phys. Rev. B 66, 020513-1 - 020513-4 (2002). H. J. Choi, M. L. Cohen, and S. G. Louie, Physica C 385, 66-74 (2003)

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