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A general computational approach for tailoring superconducting properties in BCS systems[1] JIN-CHENG ZHENG, YIMEI ZHU, Brookhaven National Laboratory, Upton, NY 11973 — We present a general computational approach for tailoring superconducting properties, such as by varying transition temperature, energy gap, critical field, in the framework of BCS theory. The relative changes in superconducting properties due to chemical doping, hydrostatic pressure, and strain fields are studied in terms of electronic and phonon contributions in a unique way that these components can be easily computed by first principles calculations based on density functional theory. Several rules for tailoring superconducting properties are derived. Some typical examples including niobium compounds and magnesium diborides and related materials will be given to illustrate the applications of these rules.

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