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First-principles calculations have been widely used for ideal crystals to design functional materials. However, various defects, which breaks the three-dimensional periodicity of ideal crystals, exist in real materials and govern their physical properties. In this study, I performed the first-principles calculations to design new electronic and thermal functional materials with incorporating both the statistic and dynamical defects on the material systems of the layered alkaline earth transition metal nitrides (*AETM*N_2), the ultra-widegap alkaline earth oxides (*AE*O), strontium titanate ($SrTiO_3$), and tin selenide (SnSe). I theoretically clarified that the issue of the unintentional high carrier generation in layered $SrTiN_2$ semiconductor would originate from the oxygen (O) impurity incorporation at the nitrogen (N) sites even at the N-rich condition, and the alkaline earth (*AE*) ion and transition metal (*TM*) ion substitutions are effective to suppress the O impurity incorporation in *AETM*N_2. I clarified the reason for the unusual hole generation by isovalent Te ion doping in SnSe, showing that it is easier to form the hole-donating Sn vacancy due to the elongated and weak Sn–Te bond in $Sn(Se_{1-x}Te_x)$ lattice, and the origin for κ_{Lat} reduction by Te doping in SnSe, which is the phonon softening and stronger phonon scattering induced by the weak chemical bond strength of Sn–Te bond.