|  |  |  |  |
| --- | --- | --- | --- |
| **Thermoelectric materials** | **zT** | **Temperature(K)** | **Ref.** |
| Sb2Te3 | | | |
| Bi0.5Sb1.5Te3 | 1.86 | 320 | 1 |
| Bi0.4Sb1.6Te3 | 1.8 | 316 | 2 |
| Bi0.45Sb1.55Te3 | 1.75 | 270 | 3 |
| Bi2Te2.7Se0.3 | 1.23 | 480 | 4 |
| (Bi2Te3)0.2(Sb2Te3)0.8 | 1.27 | 363 | 5 |
| Bi2Te2.3Se0.7 | 1.2 | 445 | 6 |
| Bi0.3Sb1.7Te3 | 1.3 | 380 |
| Bi0.5Sb1.5Te3 | 1.5 | 323 | 7 |
| Bi0.5Sb1.5Te3 + 0.1 wt.% Cu | 1.35 | 400 | 8 |
| Bi0.5Sb1.5Te3 | 1.36 | 360 | 9 |
| Bi0.4Sb1.6Te3+ 1.5 wt% β-Zn4Sb3 | 1.44 | 423 | 10 |
| Bi0.4Sb1.6Te3 | 1.36 | 400 | 11 |
| Bi0.3Sb1.625In0.075Te3 | 1.4 | 500 | 12 |
| Bi0.5Sb1.5Te3 | 1.3 | 300 | 13 |
| Bi2Te2.86 | 1.1 | 420 | 14 |
| Bi2Te3 | 0.97 | 420 | 15 |
| Bi2Te2.41Se0.6 | 1.0 | 400 | 16 |
| Bi0.4Sb1.6Te3-ZnO | 1.5 | 360 | 17 |
| Bi2Te2.4Se0.6 | 1.07 | 338 | 18 |
| Bi2Te3 +2.0 vol% AgNPs | 0.77 | 475 | 19 |
| Bi0.36Sb1.64Te3+0.4vol.% RGO | 1.16 | 393 | 20 |
| 1 vol% Ti3C2T*x*/BST | 1.23 | 400 | 21 |
| Zintls | | | |
| YbCd1.85Mn0.15Sb2 | 1.14 | 650 | 22 |
| Ca4.75Na0.25Al2Sb6 | 0.6 | 1050 | 23 |
| Sr3Ga0.93Zn0.07Sb3 | 0.9 | 1000 | 24 |
| Mg3Sb1.8Bi0.2 | 0.6 | 750 | 25 |
| Ca5Ga2As6 | 0.95 | 30 | 26 |
| YbZn0.4Cd1.6Sb2 | 1.26 | 700 | 27 |
| Yb0.99Zn2Sb2 | 0.85 | 773 | 28 |
| Yb14MgSb11 | 1.02 | 1075 | 29 |
| Mg3Sb1.8Bi0.2/GNS | 1.35 | 773 | 30 |
| Na2.19Ga2.19Sn3.81 | 1.4 | 386 | 31 |
| Mg3.2Sb1.5Bi0.49Te0.01 | 1.51 | 716 | 32 |
| Eu0.2Yb0.2Ca0.6Mg2Bi2 | 1.3 | 873 | 33 |
| Ca0.5Yb0.5Mg2Bi2 | 1.0 | 873 | 34 |
| Mg3.07Sb1.5Bi0.48Se0.02 | 1.23 | 725 | 35 |
| CaZn0.4Ag0.18Sb | 1.0 | 1073 | 36 |
| Mg3.175Mn0.025Sb1.5Bi0.49Te0.01 | 1.85 | 723 | 37 |
| Mg3.025Sb1.5Bi0.49Te0.01 | 1.6 | 770 | 38 |
| Eu2Zn0.98Sb2 | 1.0 | 823 | 39 |
| Mg3.2Pr0.02Sb1.5Bi0.5 | 1.70 | 725 | 40 |
| Ba0.7975Yb0.2Na0.0025Cd2Sb2 | 0.9 | 700 | 41 |
| Mg3.02Y0.02Sb1.5Bi0.5 | 1.8 | 773 | 42 |
| SnTe | | | |
| SnTe+4.58% CdTe coating on grains | 1.9 | 929 | 43 |
| Sn0.86Mn0.14Te(Cu2Te)0.05  Sn0.89Mn0.14Te(Cu2Te)0.05 | 1.6 | 925 | 44 |
| Sn0.92Ca0.08In0.04Te | 1.65 | 840 | 45 |
| In0.0025Sn0.9975Te | 1.1 | 873 | 46 |
| SnBi2Te4 | 0.33 | 383 | 47 |
| SnCd0.03Te-2%CdS | 1.3 | 873 | 48 |
| Sn0.98Bi0.02Te–3%HgTe | 1.35 | 910 | 49 |
| Sn0.88Mn0.12Te | 1.3 | 900 | 50 |
| Sn0.97In0.015Cd0.015Te-3%CdS | 1.4 | 923 | 51 |
| Sn0.94Ca0.09Te | 1.35 | 873 | 52 |
| Sn0.915Mn0.11In0.005Te | 1.15 | 823 | 53 |
| Sn0.93Cd0.04Te | 1.65 | 750 | 54 |
| Sn0.91Mg0.12Te(Cu2Te)0.05 | 1.4 | 900 | 55 |
| Sn0.97Bi0.03Te-3% SrTe | 1.2 | 823 | 56 |
| Sn0.83Ge0.05Mn0.2Te(Cu2Te)0.05 | 1.9 | 900 | 57 |
| (Sn0.74Ge0.2Pb0.1)0.75Mn0.275Te | 1.42 | 900 | 58 |
| Sn0.98Cd0.06Te0.88Se0.12 | 1.7 | 900 | 59 |
| Sn0.57Sb0.13Ge0.3Te | 1.6 | 721 | 60 |
| Sn1.03Te0.85Se0.075S0.075 - 2% Ag & 2% In | 1.3 | 854 | 61 |
| Sn0.48Cd0.02Ge0.25Pb0.25Te | 1.4 | 873 | 62 |
| SnTe-CdSe | 1.3 | 850 | 63 |
| (SnTe)0.9(CdSe)0.1 | 1.1 | 850 | 64 |
| Sn0.96In0.04Te–5% Cu1.75Se | 1.7 | 823 | 65 |
| (SnTe)2.94(In2Te3)0.02–(Cu2Te)0.18 | 1.55 | 873 | 66 |
| Sn0.98Pd0.025In0.025Te | 1.51 | 800 | 67 |
| SnTe + 10% MnO2 | 1.5 | 873 | 68 |
| Sn0.92Ge0.04Sb0.04Te–5% Cu2Te | 1.5 | 873 | 69 |
| PbTe | | | |
| Na0.03Eu0.03Sn0.02Pb0.92Te | 2.6 | 850 | 70 |
| Pb0.98Na0.02Te + 8% SrTe | 2.5 | 923 | 71 |
| (PbTe)0.7(PbS)0.3 + 3% Na | 2.3 | 923 | 72 |
| PbTe0.85Se0.15 + 2% Na + 4% SrTe | 2.3 | 923 | 73 |
| PbTe0.7S0.3 + 2.5% K | 2.24 | 823 | 74 |
| Pb0.945Na0.025Eu0.03Te | 2.2 | 850 | 75 |
| PbTe0.8Se0.2+8% MgTe | 2.2 | 820 | 76 |
| (PbTe)0.86(PbSe)0.07(PbS)0.07+2% Na | 2.1 | 825 | 77 |
| Pb0.98Na0.02Te | 2.0 | 773 | 78 |
| PbBi0.002Te+15% Ag2Te | 2.0 | 773 | 79 |
| Pb0.953Na0.040Ge0.007Te | 1.9 | 805 | 80 |
| PbTe+12% PbS+2% Na | 1.8 | 800 | 81 |
| Pb0.98Na0.02Te0.85Se0.15 | 1.8 | 850 | 82 |
| Pb0.98Na0.02Te+4% SrTe+0.5vol SiC | 1.73 | 750 | 83 |
| Pb0.958Na0.012Cd0.03Te | 1.7 | 775 | 84 |
| Pb0.98K0.02Te0.15Se0.85 | 1.7 | 873 | 85 |
| (La0.028Pb0.972Te) 0.947 (Ag2Te) 0.053 | 1.5 | 775 | 86 |
| PbTe0.9988I0.0012 | 1.4 | 720 | 87 |
| PbTe-Na | 1.4 | 750 | 88 |
| PbTe-2% MgTe -2% Na2Te | 1.6 | 780 | 89 |
| PbTe-2% HgTe-1% Na2Te | 1.64 | 770 | 90 |
| PbTe/7% PbTe@C:Ag | 1.65 | 723 | 91 |
| Cu2Se | | | |
| Cu2S0.52Te0.48 | 2.1 | 1000 | 92 |
| Cu1.97S | 1.7 | 1000 | 93 |
| Cu1.94Al0.02Se | 2.62 | 1029 | 94 |
| Cu2Se+1mol%In | 2.6 | 850 | 95 |
| Cu2Se + 0.15 wt% graphene | 2.44 | 870 | 96 |
| Cu2Se + 0.75 wt% CNTs | 2.4 | 1000 | 97 |
| Cu2Se + 0.1 wt% carbon-coated boron nanoparticle | 2.23 | 1000 | 98 |
| Cu1.98Li0.02Se | 2.14 | 973 | 99 |
| Nano-Cu2Se | 2.1 | 973 | 100 |
| Cu2Se + 0.05 wt% SiC | 2.0 | 850 | 101 |
| Cu2Se0.92S0.08 | 2.0 | 1000 | 102 |
| Cu2Se + 0.8 wt% carbon nanodots | 1.98 | 973 | 103 |
| Cu2Se | 1.9 | 1000 | 104 |
| Cu2Se + Ag2Se | 1.85 | 800 | 105 |
| Cu2Se | 1.82 | 850 | 106 |
| Cu2-*x*Se | 1.8 | 973 | 107 |
| Cu2Te + 50% Ag2Te | 1.8 | 1000 | 108 |
| Cu1.97Ag0.03Se | 1.0 | 400 | 109 |
| Cu2Se | 1.6 | 973 | 110 |
| Cu2Se | 1.2 | 900 | 111 |
| Cu2Se | 2.3 | 400 | 112 |
| Cu2Se | 0.38 | 750 | 113 |
| Cu2Se | 1.46 | 874 | 114 |
| SnSe | | | |
| SnSe0.97Br0.03 | 2.8 | 773 | 115 |
| SnSe | 2.6 | 923 | 116 |
| (Sn0.95Pb0.05)0.99Na0.01Se | 2.5 | 773 | 117 |
| SnSe0.97Br0.03+12% PbSe | 2.4 | 723 | 118 |
| Sn0.97Na0.03Se0.9S0.1 | 2.3 | 773 | 119 |
| Sn0.94Bi0.06Se | 2.2 | 773 | 120 |
| Sn0.985Na0.015Se+2% SnSe2 | 2.2 | 773 | 121 |
| Sn0.98Pb0.01Zn0.01Se | 2.2 | 873 | 122 |
| SnSe0.95+3% PbBr2 | 2.1 | 770 | 123 |
| Sn0.98Na0.02Se0.98Te0.02 | 2.1 | 793 | 124 |
| Sn0.95Se | 2.1 | 873 | 125 |
| Sn0.97Ge0.03Se | 2.1 | 873 | 126 |
| Sn0.985Na0.015Se | 2.0 | 773 | 127 |
| Sn0.97Na0.03Se | 2.0 | 800 | 128 |
| Sn0.99Pb0.01Se+Se QDs | 2.0 | 873 | 129 |
| Sn0.99Pb0.01Se0.93S0.07 | 1.85 | 873 | 130 |
| Sn0.978Ag0.007S0.25Se0.75 | 1.75 | 823 | 131 |
| SnSe | 1.7 | 758 | 132 |
| Sn0.948Cd0.023Se | 1.7 | 823 | 133 |
| Nanoporous SnSe | 1.7 | 823 | 134 |
| Sn0.99Ag0.01Se0.85S0.15 | 1.7 | 823 | 135 |
| SnSe + 1% PbSe | 1.7 | 873 | 136 |
| Chalcopyrite | | | |
| CuGaTe2 | 1.4 | 950 | 137 |
| AgGa0.93Te2 | 1.05 | 873 | 138 |
| Ag1.02InSe2 | 1.1 | 900 | 139 |
| Cu0.7Ag0.3Ga0.4In0.6Te2 | 1.64 | 873 | 140 |
| Cu0.7Ga0.3Te2 | 1.0 | 750 | 141 |
| Cu0.98GaSb0.02Te2 | 1.07 | 721 | 142 |
| CuGa0.36In0.64Te2 | 0.91 | 701 | 143 |
| CuGa0.99Mn0.01Te2 | 0.83 | 870 | 144 |
| CuGaTe2/3 vol% Cu2Se | 1.2 | 834 | 145 |
| (CuInTe2)0.99(2ZnTe)0.01 & 0.1% TiO2 NFs | 1.47 | 823 | 146 |
| Ag0.95GaTe2 | 0.77 | 850 | 147 |
| Cu0.89Ag0.2In0.91Te2 | 1.6 | 850 | 148 |
| Cu18Ga25Sb2.5Te47.5 | 1.2 | 854 | 149 |
| CuInTe2 | 1.18 | 850 | 150 |
| Cu0.9InTe2 | 0.54 | 710 | 151 |
| CuGaTe2 | 0.86 | 719 | 152 |
| Cu0.97Fe1.03S2 | 0.33 | 700 | 153 |
| Ag0.99In1.01Se2+1% mol Na | 0.74 | 800 | 154 |
| (Cu0.85Ag0.15InTe2)0.98(In2Te3)0.02 | 1.1 | 840 | 155 |
| CuGaTe2 | 1.0 | 900 | 156 |
| Cu2CoSnSe4 | 0.7 | 850 | 157 |
| Cu0.92Zn0.08FeS2 | 0.26 | 630 | 158 |
| Cu0.75Ag0.2InTe2 | 1.3 | 850 | 159 |
| Cu0.98In0.98Zn0.04Te2 | 0.69 | 737 | 160 |
| Ag0.9InZn0.1Se2 | 1.05 | 815 | 161 |
| (GeTe)5.5AgIn0.5Sb0.5Te2 | 0.75 | 573 | 162 |
| CuGaTe2 | 0.6 | 850 | 163 |
| Cu2.9Ga5Mn0.1Te9 | 0.81 | 804 | 164 |
| Cu0.8Ag0.2In3Se4.9Te0.1 | 0.5 | 930 | 165 |
| Cu1.95Sb0.05Ga4Te7 | 0.58 | 803 | 166 |
| Cu2.88Ga4Sb0.6Te8 | 1.51 | 870 | 167 |
| Cu3.3In4.7Ga0.3Te9 | 0.8 | 822 | 168 |
| Cu25Ga26Te49 | 0.6 | 750 | 169 |
| Cu(In0.25Ga0.75)0.99Zn0.01Te2 | 1.3 | 865 | 170 |
| Cu0.88Ag0.12FeS2 | 0.45 | 723 | 171 |
| CuGa0.98Fe0.02Te2 | 0.92 | 870 | 172 |
| Cu0.985Ni0.015InTe2 | 0.35 | 675 | 173 |
| CuGaTe2 | 1.0 | 840 | 174 |
| CuInTe2 + 6% ZnS | 1.52 | 823 | 175 |
| CuGaTe2 | 1.2 | 973 | 176 |
| CuInTe2+0.5% SnO2 | 1.1 | 823 | 177 |
| GeTe | | | |
| Ge0.86Pb0.1Bi0.04Te | 2.4 | 600 | 178 |
| Ge0.95Bi0.05Te1.025 | 2.4 | 773 | 179 |
| (GeTe)17Sb2Te3 | 2.4 | 773 | 180 |
| Ge0.9Sb0.1Te | 2.35 | 800 | 181 |
| Ge0.89Sb0.1In0.01Te | 2.3 | 650 | 182 |
| Ge0.76Sb0.08Pb0.12Te | 2.3 | 800 | 183 |
| Ge0.87Pb0.13Te | 2.25 | 673 | 184 |
| (GeTe)0.937(Bi2Se0.2Te2.8)0.063 | 2.25 | 723 | 185 |
| (Ge0.988Re0.012Te)12Sb2Te3 | 2.25 | 773 | 186 |
| (GeTe)0.73(PbSe)0.27 | 2.25 | 800 | 187 |
| Ge0.89Cr0.03Sb0.08Te | 2.2 | 780 | 188 |
| Ge0.9Cd0.05Bi0.05Te | 2.2 | 650 | 189 |
| Ge0.93Bi0.07Te1.005I0.03 | 2.2 | 723 | 190 |
| (GeTe)17Sb2Te3 + 1.5% BiI3 | 2.2 | 723 | 191 |
| Ge0.89Ti0.03Sb0.08Te | 2.2 | 725 | 192 |
| Ge0.9Sb0.1Te0.9Se0.05S0.05 | 2.1 | 630 | 193 |
| Ge0.93In0.01Bi0.06Te | 2.1 | 723 | 194 |
| Ge0.94Bi0.06Te + 0.2% nano-SiC | 2.1 | 723 | 195 |
| Ge0.84In0.01Pb0.1Sb0.05Te0.997I0.003 | 2.1 | 800 | 196 |
| Ge0.89Cu0.06Sb0.08Te | 2.03 | 750 | 197 |
| (Ge0.87Pb0.13Te)0.97(Bi2Te3)0.03 | 2.03 | 773 | 198 |
| Ge0.92Cr0.03Bi0.05Te | 2.0 | 623 | 199 |
| Sb0.1Ge0.9Te0.88Se0.12 | 2.0 | 700 | 200 |
| Ge0.99Bi0.05Te | 2.0 | 650 | 201 |
| Ge0.90Ga0.02Sb0.08Te | 1.95 | 723 | 202 |
| Ge0.8Pb0.1Bi0.1Te1.06 | 1.92 | 673 | 203 |
| (Ge0.87Pb0.13Te)0.93(Bi2Te3)0.07 | 1.9 | 573 | 204 |
| Ge0.94Bi0.06Te | 1.9 | 723 | 205 |
| Ge0.9Bi0.1Te | 1.9 | 740 | 206 |
| Ge0.9Sb0.1Te1.03 | 1.9 | 760 | 207 |
| Ge0.9Sb0.1Te | 1.85 | 725 | 208 |
| Ge0.85Mg0.05Sb0.1Te | 1.84 | 800 | 209 |
| Ge0.85Sb0.10Bi0.05Te | 1.8 | 725 | 210 |
| Ge0.89Cd0.03Sb0.08Te | 1.8 | 700 | 211 |
| Ge0.95Bi0.05Te + 5% AgBiSe2 | 1.7 | 640 | 212 |
| (AgSbTe2)10(GeTe)90 | 1.08 | 723 | 213 |
| (Ag0.6SbTe1.8)15(GeTe)85 | 1.6 | 750 | 214 |
| 0.67% Cu-doped (GeTe)0.95 (BiTe)0.05 | 1.55 | 623 | 215 |
| (GeTe)0.15 (Mn0.6Sn0.4Te)0.85 | 1.57 | 770 | 216 |
| Pb0.25Sn0.25Ge0.5Te | 1.8 | 673 | 217 |
| AgSbTe2 | | | |
| AgBi0.05Sb0.95Te2 | 1.04 | 570 | 218 |
| Ag25Sb25Se10Te40  Ag25Sb25Se5Te45 | 1.4 | 680 | 219 |
| Ag0.9SbMn0.1Te2.05 | 1.2 | 573 | 220 |
| Ag0.95Sb0.95Mn0.1Te2 | 0.74 | 550 | 221 |
| AgSb0.96Zn0.04Te2 | 1.9 | 585 | 222 |
| AgSn5SbTe7 | 1.2 | 800 | 223 |
| AgSb0.97Sn0.03Te2 | 1.1 | 600 | 224 |
| (Ag0.366Sb0.558Te)0.8(SnTe)0.2 | 0.9 | 550 | 225 |
| AgSn4SbTe6 | 1.0 | 710 | 226 |
| AgSbTe1.85Se0.15 | 2.1 | 575 | 227 |
| AgSbTe2 | 1.55 | 533 | 228 |
| AgSb0.98Bi0.02Se2 | 1.15 | 680 | 229 |
| AgSb0.93In0.07Te2 | 1.35 | 650 | 230 |
| AgSbSe2+2 mol% ZnSe | 1.1 | 635 | 231 |
| AgSb0.98Cd0.02Se2 | 1.0 | 640 | 232 |
| AgSb0.99Se2 | 1.0 | 610 | 233 |
| AgSbSe0.02Te1.98 | 1.37 | 565 | 234 |
| Ag0.99Na0.01SbTe2.02 | 1.50 | 570 | 235 |
| Ag0.96Nb0.04BiSe2 | 1.0 | 773 | 236 |
| Ag(Sb0.99La0.01)Te2 | 1.5 | 573 | 237 |
| AgSbTe2 | 1.0 | 650 | 238 |
| AgSbTe2 | 1.22 | 593 | 239 |
| AgSbTe2.01 | 1.4 | 560 | 240 |
| AgSbTe2 | 0.86 | 475 | 241 |
| Skutterudites | | | |
| Ba0.08La0.05Yb0.04Co4Sb12 | 1.7 | 850 | 242 |
| Yb0.3Ca0.1Al0.1Ga0.1In0.1Co3.75Fe0.25Sb12 | 1.0 | 773 | 243 |
| Ba0.21Co3.96Sb12Ag0.09 | 1.0 | 823 | 244 |
| Yb0.2Ce0.15In0.2Co4Sb12 | 1.43 | 800 | 245 |
| CoSb3 | 1.2 | 800 | 246 |
| In0.27Co4Sb11.9 | 1.2 | 750 | 247 |
| Ba0.3Co4Sb12 +0.5% P25+0.5% TiO2 | 1.2 | 813 | 248 |
| Ba0.3Yb0.3Fe0.4Co3.6Sb12 | 1.35 | 800 | 249 |
| (Sr,Ba,Yb)yCo4Sb12+9.1wt.% In0.4Co4Sb12 | 1.8 | 823 | 250 |
| Yb0.27Co4Sb12/0.72 vol% rGO | 1.51 | 850 | 251 |
| Yb0.3Co4Sb12+20% Sb | 1.4 | 800 | 252 |
| 0.5 vol% MWCNT-Yb0.3Co4Sb12 | 1.43 | 875 | 253 |
| (Mm,Sm)yCo4Sb12+0.5wt.% Ta0.8Zr0.2B | 1.5 | 820 | 254 |
| In0.12Yb0.2Co4Sb11.84 | 1.48 | 800 | 255 |
| 0.5 vol% SiC/Yb0.3Co4Sb12 | 1.42 | 850 | 256 |
| Ba0.15Yb0.3Co4Sb12+20%Sb | 1.53 | 823 | 257 |
| (Yb0.3Ca0.1Al0.1Ga0.1In0.1Fe0.25Co3.75Sb12)0.5(Yb0.1Ca0.1Al0.1Ga0.1In0.1Fe0.25Co3.75Sb12) | 1.3 | 773 | 258 |
| Yb0.4Co3.8Fe0.2Sb12 | 1.34 | 780 | 259 |
| Yb0.3Co4Sb11.85Sn0.15 | 1.4 | 823 | 260 |
| Ba0.3In0.3Co4Sb12+0.2% Co | 850 | 850 | 261 |
| Ba0.3In0.3Co4Sb12+0.35% BaF12O19 | 1.75 | 773 | 262 |
| Half-Heuslels | | | |
| Zr0.7Hf0.3NiSn | 1.2 | 873 | 263 |
| Ti0.5Zr0.5NiSn0.98Sb0.02 | 1.2 | 823 | 264 |
| (Hf0.25Zr0.75)0.995Nb0.005NiSn | 0.9 | 973 | 265 |
| Ti0.37Zr0.37Hf0.26NiSn | 1.0 | 725 | 266 |
| FeNb0.84Hf0.1Ti0.06Sb | 1.32 | 1200 | 267 |
| Ti0.5Hf0.5CoSb0.8Sn0.2 | 0.9 | 973 | 268 |
| FeNb0.8Ti0.2Sb | 1.1 | 1100 | 269 |
| Ti0.25Hf0.75CoSb0.85Sn0.15 | 1.2 | 983 | 270 |
| Hf0.5Zr0.5NiSn0.99Sb0.01 | 1.0 | 873 | 271 |
| Hf0.6Zr0.4NiSn0.995Sb0.005 | 1.05 | 900 | 272 |
| Hf 0.75Zr0.25NiSn0.99Sb0.01 | 1.0 | 923 | 273 |
| FeNb0.88Hf0.12Sb | 1.5 | 1500 | 274 |
| Half-Heusler | 0.8 | 973 | 275 |
| ZrCoBi0.65Sb0.15Sn0.20 | 1.42 | 973 | 276 |
| Hf0.65Zr0.35Ni0.95Pt0.05Sn0.98Sb0.02 | 0.75 | 875 | 277 |
| (Nb0.64Ta0.36)0.8Ti0.2 | 1.6 | 1200 | 278 |
| Ti0.8Hf0.2Fe0.6Ni0.4Sb | 1.0 | 973 | 279 |
| (Hf0.3Zr0.7)0.88Nb0.12CoSb | 0.85 | 1123 | 280 |
| BiCuSeO | | | |
| BiCuSeO+5% Cd | 0.98 | 923 | 281 |
| Bi0.94Pb0.06CuSeO | 1.14 | 823 | 282 |
| Bi0.925Ca0.075CuSeO | 0.8 | 773 | 283 |
| Bi0.985Na0.015CuSeO | 0.91 | 923 | 284 |
| Bi0.875Ba0.125CuSeO | 1.1 | 923 | 285 |
| BiCu0.975SeO | 0.81 | 923 | 286 |
| Bi0.925Ca0.075CuSeO. | 0.9 | 923 | 287 |
| BiCuSeO | 1.4 | 923 | 288 |
| BiCu0.9Zn0.1SeO | 0.9 | 873 | 289 |
| Bi0.96Pb0.04CuSeO | 0.91 | 873 | 290 |
| Bi0.875Ba0.125CuSeO | 1.4 | 923 | 291 |
| Bi0.94Pb0.06CuSeO | 1.2 | 923 | 292 |
| Bi0.92Na0.08CuSeO | 0.97 | 873 | 293 |
| Bi0.88Ca0.06Pb0.06CuSeO | 1.5 | 873 | 294 |
| Bi0.90Pb0.10Cu0.90Ni0.10SeO | 1.08 | 873 | 295 |
| Bi0.92Er0.08CuSeO | 0.99 | 874 | 296 |
| Bi0.9Li0.1Cu0.9Mn0.1SeO | 0.9 | 873 | 297 |
| Bi0.96Pb0.04CuSe0.95Te0.05O | 1.2 | 873 | 298 |
| Bi0.92La0.02Pb0.06CuSeO | 0.9 | 873 | 299 |
| Bi0.86Pb0.14CuSeO | 1.3 | 873 | 300 |
| Pb0.06Bi0.94Cu0.94Ag0.06SeO | 1.03 | 873 | 301 |
| Clathrates | | | |
| Ba8Ga15.967Cu0.033Sn30 | 1.35 | 540 | 302 |
| Ba8Ga16Sn30 | 1.45 | 500 | 303 |
| Ba8Ga15.9Sn30.03Ge0.07 | 0.87 | 0.87 | 304 |
| Ba8Ni0.22Zn7.22Ge37.12Sn1.44 | 0.87 | 830 | 305 |
| K8Ba16Ga40Sn96 | 0.93 | 637 | 306 |
| Ba8Zn7.66Ge36.55Sn1.79 | 0.82 | 850 | 307 |
| Ba8Ga15.9Zn0.007Sn30.1 | 1.07 | 500 | 308 |
| (K, Ba)24(Ga, Sn)136 | 1.19 | 630 | 309 |
| Ba8Ga15.7In0.2Sn30.1 | 1.05 | 540 | 310 |
| Ba8Ga16Ge30 | 1.14 | 773 | 311 |
| Ba8Cu14Ge6P26 | 0.63 | 812 | 312 |
| Ba8Ga16Ge30 | 1.1 | 823 | 313 |
| Sr7.92Ga15.04Sn0.35Ge30.69 | 1.0 | 750 | 314 |
| Ba8Ga16Ge30 | 1.0 | 773 | 315 |
| Ba8Ga16Zn1.5Sn30 | 0.63 | 537 | 316 |
| Ba8Ga16.7Sn28.6Sb0.7 | 1.0 | 480 | 317 |
| Ba8Ga10Al6Sn30 | 1.2 | 500 | 318 |
| Ba8Ga16Si30 | 0.55 | 900 | 319 |
| Ba8Ga16.9Sn19.8Ge9.3 | 0.63 | 600 | 320 |
| Ba8Ga10Al6Sn30 | 1.2 | 500 | 321 |

References

1. Kim, S. I.; Lee, K. H.; Mun, H. A.; Kim, H. S.; Hwang, S. W.; Roh, J. W.; Yang, D. J.; Shin, W. H.; Li, X. S.; Lee, Y. H.; et al. Dense Dislocation Arrays Embedded in Grain Boundaries for High-Performance Bulk Thermoelectrics. *Science* 2015, **348**, 109-114.
2. Fan, S.; Zhao, J.; Guo, J.; Yan, Q.; Ma, J.; Hng, H. H. p-Type Bi0.4Sb1.6Te3 Nanocomposites with Enhanced Figure of Merit. *Appl. Phys. Lett.* 2010, **96**, 182104.
3. Liu, C. J.; Lai, H. C.; Liu, Y. L.; Chen, L. R. High Thermoelectric Figure-of-Merit in p-Type Nanostructured (Bi,Sb)2Te3 Fabricated via Hydrothermal Synthesis and Evacuated-and-Encapsulated Sintering. *J. Mater. Chem.* 2012, **22**, 4825-4831.
4. Hong, M.; Chasapis, T. C.; Chen, Z.-G.; Yang, L.; Kanatzidis, M. G.; Snyder, G. J.; Zou, J. n-Type Bi2Te3‑*x*Se*x* Nanoplates with Enhanced Thermoelectric Efficiency Driven by Wide-Frequency Phonon Scatterings and Synergistic Carrier Scatterings. *ACS Nano* 2016, **10**, 4719-4727.
5. Dou, Y.; Qin, X.; Li, D.; Li, L.; Zou, T.; Wang, Q. Enhanced Thermopower and Thermoelectric Performance through Energy Filtering of Carriers in (Bi2Te3)0.2(Sb2Te3)0.8 Bulk Alloy Embedded with Amorphous SiO2 Nanoparticles. J*. Appl. Phys.* 2013, **114**, No. 044906.
6. Hu, L.; Zhu, T.; Liu, X.; Zhao, X. Point Defect Engineering of High-Performance Bismuth-Telluride-Based Thermoelectric Materials. *Adv. Funct. Mater.* 2014, **24**, 5211-5218.
7. Jiang, Q.; Yan, H.; Khaliq, J.; Ning, H.; Grasso, S.; Simpson, K.; Reece, M. J. Large ZT Enhancement in Hot Forged Nanostructured p-Type Bi0.5Sb1.5Te3 Bulk Alloys. *J. Mater. Chem. A* 2014, **2**, 5785-5790.
8. Lee, K.-H.; Kim, H.-S.; Kim, S.-I.; Lee, E.-S.; Lee, S.-M.; Rhyee, J.-S.; Jung, J.-Y.; Kim, I.-H.; Wang, Y.; Koumoto, K. Enhancement of Thermoelectric Figure of Merit for Bi0.5Sb1.5Te3 by Metal Nanoparticle Decoration. *J. Electron. Mater.* 2012, **41**, 1165-1169.
9. Nguyen, P.; Lee, K.; Moon, J.; Kim, S.; Ahn, K.; Chen, L.; Lee, S.; Chen, R.; Jin, S.; Berkowitz, A. Spark Erosion: A High Production Rate Method for Producing Bi0.5Sb1.5Te3 Nanoparticles with Enhanced Thermoelectric Performance. *Nanotechnology* 2012, **23**, 415604.
10. Xiao, Y.; Yang, J.-y.; Jiang, Q.-h.; Fu, L.-w.; Luo, Y.-b.; Liu, M.; Zhang, D.; Zhang, M.-y.; Li, W.-x.; Peng, J.-y.; Chen, F.-q. A Simultaneous Increase in the ZT and the Corresponding Critical Temperature of p-Type Bi0.4Sb1.6Te3 by a Combined Strategy of Dual Nanoinclusions and Carrier Engineering. *J. Mater. Chem. A* 2014, **2**, 20288-20294.
11. Xu, Z.; Hu, L.; Ying, P.; Zhao, X.; Zhu, T. Enhanced Thermoelectric and Mechanical Properties of Zone Melted p-Type (Bi,Sb)2Te3 Thermoelectric Materials by Hot Deformation. *Acta Mater.* 2015, **84**, 385-392.
12. Xu, Z.; Wu, H.; Zhu, T.; Fu, C.; Liu, X.; Hu, L.; He, J.; He, J.; Zhao, X. Attaining High Mid-Temperature Performance in (Bi,Sb)2Te3 Thermoelectric Materials via Synergistic Optimization. *NPG Asia Mater.* 2016, **8**, No. e302.
13. Zhu, T.; Xu, Z.; He, J.; Shen, J.; Zhu, S.; Hu, L.; Tritt, T. M.; Zhao, X. Hot Deformation Induced Bulk Nanostructuring of Unidirectionally Grown p-Type (Bi,Sb)2Te3 Thermoelectric Materials. *J. Mater. Chem. A* 2013, **1**, 11589-11594.
14. Wang, Y.; Liu, W.-D.; Shi, X.-L.; Hong, M.; Wang, L.-J.; Li, M.; Wang, H.; Zou, J.; Chen, Z.-G. Enhanced Thermoelectric Properties of Nanostructured n-Type Bi2Te3 by Suppressing Te Vacancy through Non-Equilibrium Fast Reaction. *Chem. Eng. J.* 2020, 391, 123513.
15. Wang, Y.; Liu, W.; Gao, H.; Wang, L.; Li, M.; Shi, X.-L.; Hong, M.; Wang, H.; Zou, J.; Chen, Z.-G. High Porosity in Nanostructured n-Type Bi2Te3 Obtaining Ultralow Lattice Thermal Conductivity. *ACS Appl. Mater. Interfaces* 2019, **11**, 31237-31244.
16. Hao, F.; Xing, T.; Qiu, P.; Hu, P.; Wei, T.; Ren, D.; Shi, X.; Chen, L. Enhanced Thermoelectric Performance in n-Type Bi2Te3-Based Alloys via Suppressing Intrinsic Excitation. *ACS Appl. Mater. Interfaces* 2018, **10**, 21372-21380.
17. Kim, K.-C.; Lim, S.-S.; Lee, S. H.; Hong, J.; Cho, D.-Y.; Mohamed, A. Y.; Koo, C. M.; Baek, S.-H.; Kim, J.-S.; Kim, S. K. Precision Interface Engineering of an Atomic Layer in Bulk Bi2Te3 Alloys for High Thermoelectric Performance. *ACS Nano* 2019, 13, 7146-7154.
18. Meroz, O.; Elkabets, N.; Gelbstein, Y. Enhanced Thermoelectric Properties of n-Type Bi2Te3‑*x*Se*x* Alloys following Melt-Spinning. *ACS Appl. Energy Mater.* 2020, **3**, 2090-2095.
19. Zhang, Q.; Ai, X.; Wang, L.; Chang, Y.; Luo, W.; Jiang, W.; Chen, L. Improved Thermoelectric Performance of Silver NanoparticlesDispersed Bi2Te3 Composites Deriving from Hierarchical Two-Phased Heterostructure. *Adv. Funct. Mater.* 2015, **25**, 966-976.
20. Shin, W. H.; Ahn, K.; Jeong, M.; Yoon, J. S.; Song, J. M.; Lee, S.; Seo, W. S.; Lim, Y. S. Enhanced Thermoelectric Performance of Reduced Graphene Oxide Incorporated Bismuth-Antimony-Telluride by Lattice Thermal Conductivity Reduction. *J. Alloys Compd.* 2017, **718**, 342-348.
21. Lu, X.; Zhang, Q.; Liao, J.; Chen, H.; Fan, Y.; Xing, J.; Gu, S.; Huang, J.; Ma, J.; Wang, J.; et al. High-Efficiency Thermoelectric Power Generation Enabled by Homogeneous Incorporation of MXene in (Bi,Sb)2Te3 Matrix. *Adv. Energy Mater.* 2020, **10**, 1902986.
22. Guo, K.; Cao, Q. G.; Feng, X. J.; Tang, M. B.; Chen, H. H.; Guo, X.; Chen, L.; Grin, Y.; Zhao, J. T. Enhanced Thermoelectric Figure of Merit of Zintl Phase YbCd2‑*x*Mn*x*Sb2 by Chemical Substitution. *Eur. J. Inorg. Chem.* 2011, **2011**, 4043-4048.
23. Toberer, E. S.; Zevalkink, A.; Crisosto, N.; Snyder, G. J. The Zintl Compound Ca5Al2Sb6 for Low-Cost Thermoelectric Power Generation. *Adv. Funct. Mater.* 2010, **20**, 4375-4380.
24. Zevalkink, A.; Zeier, W. G.; Pomrehn, G.; Schechtel, E.; Tremel, W.; Snyder, G. J. Thermoelectric Properties of Sr3GaSb3 - A ChainForming Zintl Compound. *Energy Environ. Sci.* 2012, **5**, 9121-9128.
25. Bhardwaj, A.; Rajput, A.; Shukla, A.; Pulikkotil, J.; Srivastava, A.; Dhar, A.; Gupta, G.; Auluck, S.; Misra, D.; Budhani, R. Mg3Sb2-Based Zintl Compound: A Non-Toxic, Inexpensive and Abundant Thermoelectric Material for Power Generation. *RSC Adv.* 2013, **3**, 8504-8516.
26. Yan, Y. L.; Wang, Y. X.; Zhang, G. B. Electronic Structure and Thermoelectric Performance of Zintl Compound Ca5Ga2As6. *J. Mater. Chem.* 2012, **22**, 20284-20290.
27. Guo, K.; Cao, Q.; Zhao, J. Zintl Phase Compounds AM2Sb2 (A=Ca, Sr, Ba, Eu, Yb; M=Zn, Cd) and Their Substitution Variants: A Class of Potential Thermoelectric Materials. *J. Rare Earths* 2013, **31**, 1029-1038.
28. Zevalkink, A.; Zeier, W. G.; Cheng, E.; Snyder, J.; Fleurial, J.-P.; Bux, S. Nonstoichiometry in the Zintl Phase Yb1‑*δ*Zn2Sb2 as a Route to Thermoelectric Optimization. *Chem. Mater.* 2014, **26**, 5710-5717.
29. Hu, Y.; Wang, J.; Kawamura, A.; Kovnir, K.; Kauzlarich, S. M. Yb14MgSb11 and Ca14MgSb11 - New Mg-Containing Zintl Compounds and Their Structures, Bonding, and Thermoelectric Properties. *Chem. Mater.* 2015, **27**, 343-351.
30. Bhardwaj, A.; Shukla, A.; Dhakate, S.; Misra, D. Graphene Boosts Thermoelectric Performance of a Zintl Phase Compound. *RSC Adv.* 2015, **5**, 11058-11070.
31. Yamada, T.; Yamane, H.; Nagai, H. A Thermoelectric Zintl Phase Na2+*x*Ga2+*x*Sn4-*x* with Disordered Na Atoms in Helical Tunnels. *Adv. Mater.* 2015, **27**, 4708-4713.
32. Tamaki, H.; Sato, H. K.; Kanno, T. Isotropic Conduction Network and Defect Chemistry in Mg3+*δ*Sb2-Based Layered Zintl Compounds with High Thermoelectric Performance. *Adv. Mater.* 2016, **28**, 10182-10187.
33. Shuai, J.; Geng, H.; Lan, Y.; Zhu, Z.; Wang, C.; Liu, Z.; Bao, J.; Chu, C. W.; Sui, J.; Ren, Z. Higher Thermoelectric Performance of Zintl Phases(Eu0.5Yb0.5)1‑*x*Ca*x*Mg2Bi2 by Band Engineering and Strain Fluctuation. *Proc. Natl. Acad. Sci. U. S. A.* 2016, **113**, E4125-4132.
34. Shuai, J.; Liu, Z.; Kim, H. S.; Wang, Y.; Mao, J.; He, R.; Sui, J.; Ren, Z. Thermoelectric Properties of Bi-Based Zintl Compounds Ca1‑*x*Yb*x*Mg2Bi2. *J. Mater. Chem. A* 2016, **4**, 4312-4320.
35. Zhang, J.; Song, L.; Mamakhel, A.; Jørgensen, M. R. V.; Iversen, B. B. High Performance Low-Cost n-Type Se-Doped Mg3Sb2-Based Zintl Compounds for Thermoelectric Application. *Chem. Mater.* 2017, **29**, 5371-5383.
36. Zhu, M.; Wu, Z.; Liu, Q.; Zhu, T.-J.; Zhao, X.-B.; Huang, B.; Tao, X.; Xia, S.-Q. Defect Modulation on CaZn1‑*x*Ag1‑*y*Sb (0<*x*<1; 0<*y*<1) Zintl Phases and Enhanced Thermoelectric Properties with High zT Plateaus. *J. Mater. Chem. A* 2018, **6**, 11773-11782.
37. Chen, X.; Wu, H.; Cui, J.; Xiao, Y.; Zhang, Y.; He, J.; Chen, Y.; Cao, J.; Cai, W.; Pennycook, S. J.; et al. Extraordinary Thermoelectric Performance in n-Type Manganese Doped Mg3Sb2 Zintl: High Band Degeneracy, Tuned Carrier Scattering Mechanism and Hierarchical Microstructure. *Nano Energy* 2018, **52**, 246-255.
38. Shuai, J.; Ge, B.; Mao, J.; Song, S.; Wang, Y.; Ren, Z. Significant Role of Mg Stoichiometry in Designing High Thermoelectric Performance for Mg3(Sb, Bi)2-Based n-Type Zintls. *J. Am. Chem. Soc.* 2018, **140**, 1910-1915.
39. Chen, C.; Xue, W.; Li, S.; Zhang, Z.; Li, X.; Wang, X.; Liu, Y.; Sui, J.; Liu, X.; Cao, F.; et al. Zintl-Phase Eu2ZnSb2: A Promising Thermoelectric Material with Ultralow Thermal Conductivity. *Proc. Natl. Acad. Sci. U. S. A.* 2019, **116**, 2831-2836.
40. Li, J.; Jia, F.; Zhang, S.; Zheng, S.; Wang, B.; Chen, L.; Lu, G.; Wu, L. The Manipulation of Substitutional Defects for Realizing High Thermoelectric Performance in Mg3Sb2-Based Zintl Compounds. *J. Mater. Chem. A* 2019, **7**, 19316-19323.
41. Wang, X.; Li, W.; Zhou, B.; Sun, C.; Zheng, L.; Tang, J.; Shi, X.; Pei, Y. Experimental Revelation of Multiband Transport in Heavily Doped BaCd2Sb2 with Promising Thermoelectric Performance. *Mater. Today Phys.* 2019, **8**, 123-127.
42. Song, S. W.; Mao, J.; Bordelon, M.; He, R.; Wang, Y. M.; Shuai, J.; Sun, J. Y.; Lei, X. B.; Ren, Z. S.; Chen, S.; et al. Joint Effect of Magnesium and Yttrium on Enhancing Thermoelectric Properties of n-Type Zintl Mg3+*δ*Y0.02Sb1.5Bi0.5. *Mater. Today Phys.* 2019, **8**, 25-33.
43. Hwang, J.; Kim, H.; Han, M.-K.; Hong, J.; Shim, J.-H.; Tak, J.- Y.; Lim, Y. S.; Jin, Y.; Kim, J.; Park, H. Gigantic Phonon-Scattering Cross Section To Enhance Thermoelectric Performance in Bulk Crystals. *ACS Nano* 2019, **13**, 8347-8355.
44. Li, W.; Zheng, L.; Ge, B.; Lin, S.; Zhang, X.; Chen, Z.; Chang, Y.; Pei, Y. Promoting SnTe as an Eco-Friendly Solution for p-PbTe Thermoelectric via Band Convergence and Interstitial Defects. *Adv. Mater.* 2017, **29**, 1605887.
45. Bhat, D. K.; Shenoy, U. S. Enhanced Thermoelectric Performance of Bulk Tin Telluride: Synergistic Effect of Calcium and Indium Co-Doping. *Mater. Today Phys.* 2018, **4**, 12-18.
46. Zhang, Q.; Liao, B.; Lan, Y.; Lukas, K.; Liu, W.; Esfarjani, K.; Opeil, C.; Broido, D.; Chen, G.; Ren, Z. High Thermoelectric Performance by Resonant Dopant Indium in Nanostructured SnTe. *Proc. Natl. Acad. Sci. U. S. A.* 2013, **110**, 13261-13266.
47. Kuropatwa, B. A.; Kleinke, H. Thermoelectric Properties of Stoichiometric Compounds in the (SnTe)*x*(Bi2Te3)*y* System. Z. *Anorg. Allg. Chem.* 2012, **638**, 2640-2647.
48. Tan, G.; Zhao, L.-D.; Shi, F.; Doak, J. W.; Lo, S.-H.; Sun, H.; Wolverton, C.; Dravid, V. P.; Uher, C.; Kanatzidis, M. G. High Thermoelectric Performance of p-Type SnTe via a Synergistic Band Engineering and Nanostructuring Approach. *J. Am. Chem. Soc.* 2014, **136**, 7006-7017.
49. Tan, G.; Shi, F.; Doak, J. W.; Sun, H.; Zhao, L.-D.; Wang, P.; Uher, C.; Wolverton, C.; Dravid, V. P.; Kanatzidis, M. G. Extraordinary Role of Hg in Enhancing the Thermoelectric Performance of p-Type SnTe. *Energy Environ. Sci.* 2015, **8**, 267-277.
50. Tan, G.; Shi, F.; Hao, S.; Chi, H.; Bailey, T. P.; Zhao, L. D.; Uher, C.; Wolverton, C.; Dravid, V. P.; Kanatzidis, M. G. Valence Band Modification and High Thermoelectric Performance in SnTe Heavily Alloyed with MnTe. *J. Am. Chem. Soc.* 2015, **137**, 11507-11516.
51. Tan, G.; Shi, F.; Hao, S.; Chi, H.; Zhao, L. D.; Uher, C.; Wolverton, C.; Dravid, V. P.; Kanatzidis, M. G. Codoping in SnTe: Enhancement of Thermoelectric Performance through Synergy of Resonance Levels and Band Convergence. *J. Am. Chem. Soc.* 2015, **137**, 5100-5112.
52. Al Rahal Al Orabi, R.; Mecholsky, N. A.; Hwang, J.; Kim, W.; Rhyee, J. S.; Wee,D.; Fornari, M. Band Degeneracy, Low Thermal Conductivity, and High Thermoelectric Figure of Merit in SnTe-CaTe Alloys. *Chem. Mater.* 2016, **28**, 376-384.
53. Wang, L.; Tan, X.; Liu, G.; Xu, J.; Shao, H.; Yu, B.; Jiang, H.; Yue, S.; Jiang, J. Manipulating Band Convergence and Resonant State in Thermoelectric Material SnTe by Mn-In Codoping. *ACS Energy Lett.* 2017, **2**, 1203-1207.
54. Tan, X.; Shao, H.; He, J.; Liu, G.; Xu, J.; Jiang, J.; Jiang, H. Band Engineering and Improved Thermoelectric Performance in M-Doped SnTe (M = Mg, Mn, Cd, and Hg). *Phys. Chem. Chem. Phys.* 2016, **18**, 7141-7147.
55. Zheng, L.; Li, W.; Lin, S.; Li, J.; Chen, Z.; Pei, Y. Interstitial Defects Improving Thermoelectric SnTe in Addition to Band Convergence. *ACS Energy Lett.* 2017, **2**, 563-568.
56. Zhao, L.-D.; Zhang, X.; Wu, H.; Tan, G.; Pei, Y.; Xiao, Y.; Chang, C.; Wu, D.; Chi, H.; Zheng, L.; et al. Enhanced Thermoelectric Properties in the Counter-Doped SnTe System with Strained Endotaxial SrTe. *J. Am. Chem. Soc.* 2016, **138**, 2366-2373.
57. Tang, J.; Gao, B.; Lin, S.; Li, J.; Chen, Z.; Xiong, F.; Li, W.; Chen, Y.; Pei, Y. Manipulation of Band Structure and Interstitial Defects for Improving Thermoelectric SnTe. *Adv. Funct. Mater.* 2018, **28**,1803586.
58. Hu, L.; Zhang, Y.; Wu, H.; Li, J.; Li, Y.; Mckenna, M.; He, J.; Liu, F.; Pennycook, S. J.; Zeng, X. Entropy Engineering of SnTe: MultiPrincipal-Element Alloying Leading to Ultralow Lattice Thermal Conductivity and State-of-the-Art Thermoelectric Performance. *Adv. Energy Mater.* 2018, **8**, 1802116.
59. Hong, M.; Wang, Y.; Xu, S.; Shi, X.; Chen, L.; Zou, J.; Chen, Z.- G. Nanoscale Pores Plus Precipitates Rendering High-Performance Thermoelectric SnTe1‑*x*Se*x* with Refined Band Structures. *Nano Energy* 2019, **60**, 1-7.
60. Banik, A.; Ghosh, T.; Arora, R.; Dutta, M.; Pandey, J.; Acharya, S.; Soni, A.; Waghmare, U. V.; Biswas, K. Engineering Ferroelectric Instability to Achieve Ultralow Thermal Conductivity and High Thermoelectric Performance in Sn1‑*x*Ge*x*Te. *Energy Environ. Sci.* 2019, **12**, 589-595.
61. Roychowdhury, S.; Biswas, R. K.; Dutta, M.; Pati, S. K.; Biswas, K. Phonon Localization and Entropy-Driven Point Defects Lead to Ultralow Thermal Conductivity and Enhanced Thermoelectric Performance in (SnTe)1‑2*x*(SnSe)*x*(SnS)*x*. *ACS Energy Lett.* 2019, **4**, 1658-1662.
62. Xie, G.; Li, Z.; Luo, T.; Bai, H.; Sun, J.; Xiao, Y.; Zhao, L.-D.; Wu, J.; Tan, G.; Tang, X. Band Inversion Induced Multiple Electronic Valleys for High Thermoelectric Performance of SnTe with Strong Lattice Softening. *Nano Energy* 2020, **69**, 104395.
63. Ibanez, M.; Hasler, R.; Genc, A.; Liu, Y.; Kuster, B.; Schuster, M.; Dobrozhan, O.; Cadavid, D.; Arbiol, J.; Cabot, A.; et al. LigandMediated Band Engineering in Bottom-Up Assembled SnTe Nanocomposites for Thermoelectric Energy Conversion. *J. Am. Chem. Soc.* 2019, **141**, 8025-8029.
64. Gao, B.; Tang, J.; Meng, F.; Li, W. Band Manipulation for High Thermoelectric Performance in SnTe through Heavy CdSe-Alloying. *J. Materiomics* 2019, **5**, 111-117.
65. Li, D.; Ming, H. W.; Li, J. M.; Zhang, J.; Qin, X. Y.; Xu, W. High Thermoelectric Performance of SnTe via In Doping and Cu1.75Se Nanostructuring Approach. *ACS Appl. Energy Mater.* 2019, **2**, 8966-8973.
66. Guo, F.; Cui, B.; Geng, H.; Zhang, Y.; Wu, H.; Zhang, Q.; Yu, B.; Pennycook, S. J.; Cai, W.; Sui, J. Simultaneous Boost of Power Factor and Figure-of-Merit in In-Cu Codoped SnTe. *Small* 2019, **15**, e1902493.
67. Ma, Z.; Lei, J.; Zhang, D.; Wang, C.; Wang, J.; Cheng, Z.; Wang, Y. Enhancement of Thermoelectric Properties in Pd-In Co-Doped SnTe and Its Phase Transition Behavior. A*CS Appl. Mater. Interfaces* 2019, **11**, 33792-33802.
68. Zhou, Z.; Yang, J.; Jiang,Q.; Xin, J.; Li, S.; Wang, X.; Lin, X.; Chen, R.; Basit, A.; Chen, Q. Facile Route to High-Performance SnTe-Based Thermoelectric Materials: Synergistic Regulation of Electrical and Thermal Transport by In Situ Chemical Reactions. *Chem. Mater.* 2019, **31**,3491-3497.
69. Li, X.; Liu, J.; Li, S.; Zhang, J.; Li, D.; Xu, R.; Zhang, Q.; Zhang, X.; Xu, B.; Zhang, Y.; Xu, F.; Tang, G. Synergistic Band Convergence and Endotaxial Nanostructuring: Achieving Ultralow Lattice Thermal Conductivity and High Figure of Merit in Eco-friendly SnTe. *Nano Energy* 2020, **67**, 104261.

1. Wu, Y.; Chen, Z.; Nan, P.; Xiong, F.; Lin, S.; Zhang, X.; Chen,Y.; Chen, L.; Ge, B.; Pei, Y. Lattice Strain Advances Thermoelectrics. *Joule* 2019, **3**, 1276-1288.
2. Tan, G.; Shi, F.; Hao, S.; Zhao, L.-D.; Chi, H.; Zhang, X.; Uher, C.; Wolverton, C.; Dravid, V. P.; Kanatzidis, M. G. Non-Equilibrium Processing Leads to Record High Thermoelectric Figure of Merit in PbTe-SrTe. *Nat. Commun.* 2016, 7, 12167.
3. Wu, D.; Zhao, L.-D.; Tong, X.; Li, W.; Wu, L.; Tan, Q.; Pei, Y.; Huang, L.; Li, J.-F.; Zhu, Y.; et al. Superior Thermoelectric Performance in PbTe-PbS Pseudo-Binary: Extremely Low Thermal Conductivity and Modulated Carrier Concentration. *Energy Environ. Sci.* 2015, **8**, 2056-2068.
4. Pei, Y.; Tan, G.; Feng, D.; Zheng, L.; Tan, Q.; Xie, X.; Gong, S.; Chen, Y.; Li, J. F.; He, J.; et al. Integrating Band Structure Engineering with All-Scale Hierarchical Structuring for High Thermoelectric Performance in PbTe System. *Adv. Energy Mater.* 2017, **7**, 1601450.
5. Wu, H.; Zhao, L.-D.; Zheng, F.; Wu, D.; Pei, Y.; Tong, X.; Kanatzidis, M. G.; He, J. Broad Temperature Plateau for Thermoelectric Figure of Merit ZT > 2 in Phase-Separated PbTe0.7S0.3. *Nat. Commun.* 2014, **5**, 4515.
6. Chen, Z.; Jian, Z.; Li, W.; Chang, Y.; Ge, B.; Hanus, R.; Yang, J.; Chen, Y.; Huang, M.; Snyder, G. J.; Pei, Y. Lattice Dislocations Enhancing Thermoelectric PbTe in Addition to Band Convergence. *Adv. Mater.* 2017, **29**, 1606768.
7. Fu, T.; Yue, X.; Wu, H.; Fu, C.; Zhu, T.; Liu, X.; Hu, L.; Ying, P.; He, J.; Zhao, X. Enhanced Thermoelectric Performance of PbTe Bulk Materials with Figure of Merit zT > 2 by Multi-Functional Alloying. *J. Materiomics* 2016, **2**, 141-149.
8. Korkosz, R. J.; Chasapis, T. C.; Lo, S.-h.; Doak, J. W.; Kim, Y. J.; Wu, C.-I.; Hatzikraniotis, E.; Hogan, T. P.; Seidman, D. N.; Wolverton, C.; et al. High ZT in p-Type (PbTe)1‑2*x*(PbSe)*x*(PbS)*x* Thermoelectric Materials. *J. Am. Chem. Soc.* 2014, **136**, 3225-3237.
9. Wang, H.; Hwang, J.; Snedaker, M. L.; Kim, I.-h.; Kang, C.; Kim, J.; Stucky, G. D.; Bowers, J.; Kim, W. High Thermoelectric Performance of a Heterogeneous PbTe Nanocomposite. *Chem. Mater.* 2015, **27**, 944-949.
10. Lee, M. H.; Yun, J. H.; Kim, G.; Lee, J. E.; Park, S.-D.; Reith, H.; Schierning, G.; Nielsch, K.; Ko, W.; Li, A.-P.; et al. Synergetic Enhancement of Thermoelectric Performance by Selective Charge Anderson Localization-Delocalization Transition in n-Type Bi-Doped PbTe/Ag2Te Nanocomposite. *ACS Nano* 2019, **13**, 3806-3815.
11. Jood, P.; Ohta, M.; Yamamoto, A.; Kanatzidis, M. G. Excessively Doped PbTe with Ge-Induced Nanostructures Enables High-Efficiency Thermoelectric Modules. *Joule* 2018, **2**, 1339-1355.
12. Girard, S. N.; He, J.; Zhou, X.; Shoemaker, D.; Jaworski, C. M.; Uher, C.; Dravid, V. P.; Heremans, J. P.; Kanatzidis, M. G. High Performance Na-Doped PbTe-PbS Thermoelectric Materials: Electronic Density of States Modification and Shape-Controlled Nano-structures. *J. Am. Chem. Soc.* 2011, **133**, 16588-16597.
13. Pei, Y.; Shi, X.; LaLonde, A.; Wang, H.; Chen, L.; Snyder, G. J. Convergence of Electronic Bands for High Performance Bulk Thermoelectrics. *Nature* 2011, 473, 66-69.
14. Ai, X.; Hou, D.; Liu, X.; Gu, S.; Wang, L.; Jiang, W. Enhanced Thermoelectric Performance of PbTe-Based Nanocomposites through Element Doping and SiC Nanoparticles Dispersion. *Scr. Mater.* 2020, **179**, 86-91.
15. Pei, Y.; LaLonde, A. D.; Heinz, N. A.; Snyder, G. J. High Thermoelectric Figure of Merit in PbTe Alloys Demonstrated in PbTe-CdTe. *Adv. Energy Mater.* 2012, **2**, 670-675.
16. Zhang, Q.; Cao, F.; Liu, W.; Lukas, K.; Yu, B.; Chen, S.; Opeil, C.; Broido, D.; Chen, G.; Ren, Z. Heavy Doping and Band Engineering by Potassium to Improve the Thermoelectric Figure of Merit in p-Type PbTe, PbSe, and PbTe1‑*y*Se*y*. *J. Am. Chem. Soc.* 2012, **134**, 10031-10038.
17. Pei, Y.; Lensch-Falk, J.; Toberer, E. S.; Medlin, D. L.; Snyder, G. J. High Thermoelectric Performance in PbTe due to Large Nanoscale Ag2Te Precipitates and La Doping. *Adv. Funct. Mater.* 2011, **21**, 241-249.
18. LaLonde, A. D.; Pei, Y.; Snyder, G. J. Reevaluation of PbTe1‑*x*I*x* as High Performance n-Type Thermoelectric Material. *Energy Environ. Sci.* 2011, **4**, 2090-2096.
19. Pei, Y.; LaLonde, A.; Iwanaga, S.; Snyder, G. J. High Thermoelectric Figure of Merit in Heavy Hole Dominated PbTe. *Energy Environ. Sci.* 2011, **4**, 2085-2089.
20. Ohta, M.; Biswas, K.; Lo, S. H.; He, J.; Chung, D. Y.; Dravid, V. P.; Kanatzidis, M. G. Enhancement of Thermoelectric Figure of Merit by the Insertion of MgTe Nanostructures in p-Type PbTe Doped with Na2Te. *Adv. Energy Mater.* 2012, **2**, 1117-1123.
21. Ahn, K.; Biswas, K.; He, J.; Chung, I.; Dravid, V.; Kanatzidis, M. G. Enhanced Thermoelectric Properties of p-Type Nanostructured PbTe-MTe (M = Cd, Hg) Materials. *Energy Environ. Sci.* 2013, **6**, 1529-1537.
22. Xiang, B.; Liu, J.; Yan, J.; Xia, M.; Zhang, Q.; Chen, L.; Li, J.; Tan, X. Y.; Yan, Q.; Wu, Y. Local Nanostructures Enhanced the Thermoelectric Performance of n-Type PbTe. *J. Mater. Chem. A* 2019, **7**, 18458-18467.
23. He, Y.; Lu, P.; Shi, X.; Xu, F.; Zhang, T.; Snyder, G. J.; Uher, C.; Chen, L. Ultrahigh Thermoelectric Performance in Mosaic Crystals. *Adv. Mater.* 2015, **27**, 3639-3644.
24. He, Y.; Day, T.; Zhang, T.; Liu, H.; Shi, X.; Chen, L.; Snyder, G. J. High Thermoelectric Performance in Non-Toxic Earth-Abundant Copper Sulfide. *Adv. Mater.* 2014, **26**, 3974-3978.
25. Zhong, B.; Zhang, Y.; Li, W.; Chen, Z.; Cui, J.; Li, W.; Xie, Y.; Hao, Q.; He, Q. High Superionic Conduction Arising from Aligned Large Lamellae and Large Figure of Merit in Bulk Cu1.94Al0.02Se. *Appl. Phys. Lett.* 2014, **105**, 123902.
26. Olvera, A.; Moroz, N.; Sahoo, P.; Ren, P.; Bailey, T.; Page, A.; Uher, C.; Poudeu, P. Partial Indium Solubility Induces Chemical Stability and Colossal Thermoelectric Figure of Merit in Cu2Se. *Energy Environ. Sci.* 2017, **10**, 1668-1676.
27. Li, M.; Cortie, D. L.; Liu, J.; Yu, D.; Islam, S. M. K. N.; Zhao, L.; Mitchell, D. R.; Mole, R. A.; Cortie, M. B.; Dou, S.; Wang, X. Ultra-High Thermoelectric Performance in Graphene Incorporated Cu2Se: Role of Mismatching Phonon Modes. *Nano Energy* 2018, **53**, 993-1002.
28. Nunna, R.; Qiu, P.; Yin, M.; Chen, H.; Hanus, R.; Song, Q.; Zhang, T.; Chou, M.-Y.; Agne, M. T.; He, J.; et al. Ultrahigh Thermoelectric Performance in Cu2Se-Based Hybrid Materials with Highly Dispersed Molecular CNTs. *Energy Environ. Sci.* 2017, **10**, 1928-1935.
29. Li, M.; Islam, S. M. K. N.; Yahyaoglu, M.; Pan, D.; Shi, X.; Chen, L.; Aydemir, U.; Wang, X. Ultrahigh Figure-of-Merit of Cu2Se Incorporated with Carbon Coated Boron Nanoparticles. *InfoMat* 2019, **1**, 108-115.
30. Hu, Q.; Zhu, Z.; Zhang, Y.; Li, X.-J.; Song, H.; Zhang, Y. Remarkably High Thermoelectric Performance of Cu2‑*x*Li*x*Se Bulks with Nanopores. *J. Mater. Chem. A* 2018, **6**, 23417-23424.
31. Gahtori, B.; Bathula, S.; Tyagi, K.; Jayasimhadri, M.; Srivastava, A.; Singh, S.; Budhani, R.; Dhar, A. Giant Enhancement in Thermoelectric Performance of Copper Selenide by Incorporation of Different Nanoscale Dimensional Defect Features. *Nano Energy* 2015, **13**, 36-46.
32. Lei, J.; Ma, Z.; Zhang, D.; Chen, Y.; Wang, C.; Yang, X.; Cheng, Z.; Wang, Y. High Thermoelectric Performance in Cu2Se Superionic Conductor with Enhanced Liquid-Like Behaviour by Dispersing SiC. *J. Mater. Chem. A* 2019, **7**, 7006-7014.
33. Zhao, K.; Blichfeld, A. B.; Chen, H.; Song, Q.; Zhang, T.; Zhu, C.; Ren, D.; Hanus, R.; Qiu, P.; Iversen, B. B.; et al. Enhanced Thermoelectric Performance through Tuning Bonding Energy in Cu2Se1‑*x*S*x* Liquid-like Materials. *Chem. Mater.* 2017, **29**, 6367-6377.
34. Hu, Q.; Zhang, Y.; Zhang, Y.; Li, X.-J.; Song, H. High Thermoelectric Performance in Cu2Se/CDs Hybrid Materials. *J. Alloys Compd.* 2020, **813**, 152204.
35. Zhao, K.; Duan, H.; Raghavendra, N.; Qiu, P.; Zeng, Y.; Zhang, W.; Yang, J.; Shi, X.; Chen, L. Solid-State Explosive Reaction for Nanoporous Bulk Thermoelectric Materials. *Adv. Mater.* 2017, **29**, 1701148.
36. Ballikaya, S.; Sertkol, M.; Oner, Y.; Bailey, T. P.; Uher, C. Fracture Structure and Thermoelectric Enhancement of Cu2Se with Substitution of Nanostructured Ag2Se. *Phys. Chem. Chem. Phys.* 2019, **21**, 13569-13577.
37. Yang, L.; Chen, Z.-G.; Han, G.; Hong, M.; Zou, J. Impacts of Cu Deficiency on the Thermoelectric Properties of Cu2‑*x*Se Nanoplates. *Acta Mater.* 2016, **113**, 140-146.
38. Zhao, L.-l.; Wang, X.-l.; Wang, J.-y.; Cheng, Z.-x.; Dou, S.-x.; Wang, J.; Liu, L.-Q. Superior Intrinsic Thermoelectric Performance with zT of 1.8 in Single-Crystal and Melt-Quenched Highly Dense Cu2‑*x*Se Bulks. *Sci. Rep.* 2015, **5**, 7671.
39. Zhao, K.; Liu, K.; Yue, Z.; Wang, Y.; Song, Q.; Li, J.; Guan, M.; Xu, Q.; Qiu, P.; Zhu, H.; et al. Are Cu2Te-Based Compounds Excellent Thermoelectric Materials? *Adv. Mater.* 2019, **31**, 1903480.
40. Brown, D. R.; Day, T.; Borup, K. A.; Christensen, S.; Iversen, B. B.; Snyder, G. J. Phase Transition Enhanced Thermoelectric Figure of Merit in Copper Chalcogenides. *APL Mater.* 2013, **1**, No. 052107.
41. Yu, B.; Liu, W.; Chen, S.; Wang, H.; Wang, H.; Chen, G.; Ren, Z. Thermoelectric Properties of Copper Selenide with Ordered Selenium Layer and Disordered Copper Layer. *Nano Energy* 2012, **1**, 472-478.
42. Ballikaya, S.; Chi, H.; Salvador, J. R.; Uher, C. Thermoelectric Properties of Ag-Doped Cu2Se and Cu2Te. *J. Mater. Chem. A* 2013, **1**, 12478-12484.
43. Liu, H.; Yuan, X.; Lu, P.; Shi, X.; Xu, F.; He, Y.; Tang, Y.; Bai, S.; Zhang, W.; Chen, L.; et al. Ultrahigh Thermoelectric Performance by Electron and Phonon Critical Scattering in Cu2Se1‑*x*I*x*. *Adv. Mater.* 2013, **25**, 6607-6612.
44. Xiao, X.-X.; Xie, W.-J.; Tang, X.-F.; Zhang, Q.-J. Phase Transition and High Temperature Thermoelectric Properties of Copper Selenide Cu2‑*x*Se (0≤*x*≤0.25). *Chin. Phys. B* 2011, **20**, No. 087201.
45. Butt, S.; Farooq, M. U.; Mahmood, W.; Salam, S.; Sultan, M.; Basit, M. A.; Ma, J.; Lin, Y.; Nan, C.-W. One-Step Rapid Synthesis of Cu2Se with Enhanced Thermoelectric Properties. *J. Alloys Compd.* 2019, **786**, 557-564.
46. Chang, C.; Wu, M.; He, D.; Pei, Y.; Wu, C.-F.; Wu, X.; Yu, H.; Zhu, F.; Wang, K.; Chen, Y.; et al. 3D Charge and 2D Phonon Transports Leading to High Out-of-Plane ZT in n-Type SnSe Crystals. *Science* 2018, **360**, 778-783.
47. Zhao, L. D.; Lo, S. H.; Zhang, Y.; Sun, H.; Tan, G.; Uher, C.; Wolverton, C.; Dravid, V. P.; Kanatzidis, M. G. Ultralow Thermal Conductivity and High Thermoelectric Figure of Merit in SnSe Crystals. *Nature* 2014, **508**, 373-377.
48. Lee, Y. K.; Luo, Z.; Cho, S. P.; Kanatzidis, M. G.; Chung, I. Surface Oxide Removal for Polycrystalline SnSe Reveals Near-SingleCrystal Thermoelectric Performance. *Joule* 2019, **3**, 719-731.
49. Chang, C.; Wang, D.; He, D.; He, W.; Zhu, F.; Wang, G.; He, J.; Zhao, L.-D. Realizing High-Ranged Out-of-Plane ZTs in n-Type SnSe Crystals through Promoting Continuous Phase Transition. *Adv. Energy Mater.* 2019, **9**, 1901334.
50. Peng, K.; Zhang, B.; Wu, H.; Cao, X.; Li, A.; Yang, D.; Lu, X.; Wang, G.; Han, X.; Uher, C.; Zhou, X. Ultra-High Average Figure of Merit in Synergistic Band Engineered Sn*x*Na1‑*x*Se0.9S0.1 Single Crystals. *Mater. Today* 2018, **21**, 501-507.
51. Duong, A. T.; Nguyen, V. Q.; Duvjir, G.; Duong, V. T.; Kwon, S.; Song, J. Y.; Lee, J. K.; Lee, J. E.; Park, S.; Min, T.; et al. Achieving ZT = 2.2 with Bi-Doped n-Type SnSe Single Crystals. *Nat. Commun.* 2016, **7**, 13713.
52. Qin, B.; Zhang, Y.; Wang, D.; Zhao, Q.; Gu, B.; Zhang, H.; Wu, H.; Ye, B.; Pennycook, S. J.; Zhao, L.-D. Ultrahigh Average ZT Realized in p-Type SnSe Crystalline Thermoelectrics through Producing Extrinsic Vacancies. *J. Am. Chem. Soc.* 2020, **142**, 5901-5909.
53. Liu, J.; Wang, P.; Wang, M.; Xu, R.; Zhang, J.; Liu, J.; Li, D.; Liang, N.; Du, Y.; Chen, G.; Tang, G. Achieving High Thermoelectric Performance with Pb and Zn Codoped Polycrystalline SnSe via Phase Separation and Nanostructuring Strategies. *Nano Energy* 2018, **53**, 683-689.
54. Mao, L.; Yin, Y.; Zhang, Q.; Liu, G.-Q.; Wang, H.; Guo, Z.; Hu, H.; Xiao, Y.; Tan, X.; Jiang, J. Fermi-Surface Dynamics and High Thermoelectric Performance along the Out-of-Plane Direction in n-Type SnSe Crystals. *Energy Environ. Sci.* 2020, **13**, 616-621.
55. Qin, B.; Wang, D.; He, W.; Zhang, Y.; Wu, H.; Pennycook, S. J.; Zhao, L.-D. Realizing High Thermoelectric Performance in p-Type SnSe through Crystal Structure Modification. *J. Am. Chem. Soc.* 2019, **141**, 1141-1149.
56. Wei, W.; Chang, C.; Yang, T.; Liu, J.; Tang, H.; Zhang, J.; Li, Y.; Xu, F.; Zhang, Z.; Li, J.-F.; Tang, G. Achieving High Thermoelectric Figure of Merit in Polycrystalline SnSe via Introducing Sn Vacancies. *J. Am. Chem. Soc.* 2018, **140**, 499-505.
57. Chandra, S.; Biswas, K. Realization of High Thermoelectric Figure of Merit in Solution Synthesized 2D SnSe Nanoplates via Ge alloying. *J. Am. Chem. Soc.* 2019, **141**, 6141-6145.
58. Zhao, L.-D.; Tan, G.; Hao, S.; He, J.; Pei, Y.; Chi, H.; Wang, H.; Gong, S.; Xu, H.; Dravid, V. P.; et al. Ultrahigh Power Factor and Thermoelectric Performance in Hole-Doped Single-Crystal SnSe. *Science* 2016, **351**, 141-144.
59. Peng, K.; Lu, X.; Zhan, H.; Hui, S.; Tang, X.; Wang, G.; Dai, J.; Uher, C.; Wang, G.; Zhou, X. Broad Temperature Plateau for High ZTs in Heavily Doped p-Type SnSe Single Crystals. *Energy Environ. Sci.* 2016, **9**, 454-460.
60. Xu, R.; Huang, L.; Zhang, J.; Li, D.; Liu, J.; Liu, J.; Fang, J.; Wang, M.; Tang, G. Nanostructured SnSe Integrated with Se Quantum Dots with Ultrahigh Power Factor and Thermoelectric Performance from Magnetic Field-Assisted Hydrothermal Synthesis. *J. Mater. Chem. A* 2019, **7**, 15757-15765.
61. Lu, W.; Li, S.; Xu, R.; Zhang, J.; Li, D.; Feng, Z.; Zhang, Y.; Tang, G. Boosting Thermoelectric Performance of SnSe via Tailoring Band Structure, Suppressing Bipolar Thermal Conductivity, and Introducing Large Mass Fluctuation. *ACS Appl. Mater. Interfaces* 2019, **11**, 45133-45141.
62. Asfandiyar; Cai, B.; Zhuang, H.-L.; Tang, H.; Li, J.-F. Polycrystalline SnSe-Sn1‑*y*S Solid Solutions: Vacancy Engineering and Nanostructuring Leading to High Thermoelectric Performance. *Nano Energy* 2020, **69**, 104393.
63. Burton, M. R.; Mehraban, S.; Beynon, D.; McGettrick, J.; Watson, T.; Lavery, N. P.; Carnie, M. J. 3D Printed SnSe Thermoelectric Generators with High Figure of Merit. *Adv. Energy Mater.* 2019, **9**, 1900201.
64. Shi, X.; Wu, A.; Feng, T.; Zheng, K.; Liu, W.; Sun, Q.; Hong, M.; Pantelides, S. T.; Chen, Z. G.; Zou, J. High Thermoelectric Performance in p-type Polycrystalline Cd-doped SnSe Achieved by a Combination of Cation Vacancies and Localized Lattice Engineering. *Adv. Energy Mater.* 2019, **9**, 1803242.
65. Shi, X.; Wu, A.; Liu, W.; Moshwan, R.; Wang, Y.; Chen, Z.-G.; Zou, J. Polycrystalline SnSe with Extraordinary Thermoelectric Property via Nanoporous Design. *ACS Nano* 2018, **12**, 11417-11425.
66. Lin, C.-C.; Lydia, R.; Yun, J. H.; Lee, H. S.; Rhyee, J. S. Extremely Low Lattice Thermal Conductivity and Point Defect Scattering of Phonons in Ag-Doped (SnSe)1‑*x*(SnS)*x* Compounds. *Chem. Mater.* 2017, **29**, 5344-5352.
67. Tang, G.; Wei, W.; Zhang, J.; Li, Y.; Wang, X.; Xu, G.; Chang, C.; Wang, Z.; Du, Y.; Zhao, L.-D. Realizing High Figure of Merit in Phase-Separated Polycrystalline Sn1‑*x*Pb*x*Se. *J. Am. Chem. Soc.* 2016, **138**, 13647-13654.
68. Plirdpring, T.; Kurosaki, K.; Kosuga, A.; Day, T.; Firdosy, S.; Ravi, V.; Snyder, G. J.; Harnwunggmoung, A.; Sugahara, T. ; Ohishi, Y.; Muta, H.; Yamanaka, S. Chalcopyrite CuGaTe2 : A High-Efficiency Bulk Thermoelectric Material. *Adv. Mater.* 2012, **24**, 3622-3626.
69. Su, X. L.; Zhao, N.; Hao, S. Q.; Stoumpos, C. C.; Liu, M. Y.; Chen, H. J.; Xie, H. Y.; Zhang, Q. J.; Wolverton, C.; Tang, X. F.; Kanatzidis, M. G. High Thermoelectric Performance in the Wide Band-Gap AgGa1-*x*Te2 Compounds: Directional Negative Thermal Expansion and Intrinsically Low Thermal Conductivity. *Adv. Funct. Mater.* 2018, **29**, 1806534.
70. Qiu, P. F.; Qin, Y. T.; Zhang, Q. H.; Li, R. X.; Yang, J.; Song, Q. F.; Tang, Y. S.; Bai, S. Q.; Shi, X.; Chen, L. D. Intrinsically High Thermoelectric Performance in AgInSe2 n-Type Diamond-Like Compounds. *Adv. Sci.* 2017, **5**, 1700727.
71. Zhang, J.; Huang, L. L.; Zhu, C.; Zhou, C. J.; Jabar, B.; Li, J. M.; Zhu, X. G.; Wang, L.; Song, C. J.; Xin, H. X.; Li, D.; Qin, X. Y. Design of Domain Structure and Realization of Ultralow Thermal Conductivity for Record-High Thermoelectric Performance in Chalcopyrite. *Adv. Mater.* 2019, 31, 1905210.
72. Shen, J. W.; Zhang, X. Y.; Chen, Z. W.; Lin, S. Q.; Li, J.; Li, W.; Li, S. S.; Chen, Y.; Pei, Y. Z. Substitutional defects enhancing thermoelectric CuGaTe2. *J. Mater. Chem. A* 2017, **5**, 5314-5320.
73. Cui, J. L.; Li, Y. P.; Du, Z. L.; Meng, Q. S.; Zhou, H. Promising defect thermoelectric semiconductors Cu1-*x*GaSb*x*Te2 (*x*=0-0.1) with the chalcopyrite structure. *J. Mater. Chem. A* 2013, **1**, 677-683.
74. Li, Y. P.; Meng, Q. S.; Deng, Y.; Zhou, H.; Gao, Y. L.; Li, Y. Y.; Yang, J. F.; Cui, J. L. High thermoelectric performance of solid solutions CuGa1-*x*In*x*Te2 (*x*=0-1.0). *APL.* 2012, **100**, 231903.
75. Ahmed, F.; Tsujii, N.; Mori, T. Thermoelectric properties of CuGa1-*x*Mn*x*Te2: power factor enhancement by incorporation of magnetic ions. *J. Mater. Chem. A* 2017, **5**, 7545-7554.
76. Zhang, J.; Qin, X. Y.; Li, D.; Xin, H. X.; Song, C. J.; Li, L. L.; Zhu, X. G.; Wang, Z. M.; Guo, G. L.; Wang, L. Enhanced thermoelectric performance of CuGaTe2 based composites incorporated with nanophase Cu2Se. *J. Mater. Chem. A* 2014, **2**, 2891-2895.
77. Luo, Y. B.; Yang, J. Y.; Jiang, Q. H.; Li, W. X.; Xiao, Y.; Fu, L. W.; Zhang, D.; Zhou, Z. W.; Cheng, Y. D. Large enhancement of thermoelectric performance of CuInTe2 via a synergistic strategy of point defects and microstructure engineering. *Nano Energy* 2015, **18**, 37-46.
78. Yusufu, A.; Kurosaki, K.; Kosuga, A.; Sugahara, T.; Ohishi, Y.; Muta, H.; Yamanaka, S. Thermoelectric properties of Ag1-*x*GaTe2 with chalcopyrite structure. *APL.* 2011, **99**, 061902.
79. H. Y. Xie, S. Q. Hao, S. T. Cai, T. P. Bailey, C. Uher, C. Wolverton, V. P. Dravid, M. G. Kanatzidis, Ultralow thermal conductivity in diamondoid lattices: high thermoelectric performance in chalcopyrite Cu0.8+*y*Ag0.2In1-*y*Te2. *Energy Environ. Sci.* 2020, **13**, 3693-3705.
80. Zhu, J. H.; Luo, Y.; Cai, G. M.; Liu, X. L.; Du, Z. L.; Tang, F. L.; Cui, J. L. Signifificant improvement in the thermoelectric performance of Sb-incorporated chalcopyrite compounds Cu18Ga25Sb*x*Te50-*x* (*x*=0-3.125) through the coordination of energy band and crystal structures. *J. Mater. Chem. A* 2017, **5**, 24199-24207.
81. Liu, R. H.; Xi, L. L.; Liu, H. L.; Shi, X.; Zhang, W. Q.; Chen, L. D. Ternary compound CuInTe2: a promising thermoelectric material with diamond-like structure. *Chem. Commun.* 2012, **48**, 3818-3820.
82. Kosuga, A.; Plirdpring, T.; Higashine, R.; Matsuzawa, M.; Kurosaki, K.; Yamanaka, S. High-temperature thermoelectric properties of Cu1-*x*InTe2 with a chalcopyrite structure. *Appl. Phys. Lett.* 2012, **100**, 042108.
83. Wu, W. C.; Li, Y. P.; Du, Z. L.; Meng, Q. S.; Sun, Z.; Ren, W.; Cui, J. L. Manipulation of the crystal structure defects: An alternative route to the reduction in lattice thermal conductivity and improvement in thermoelectric performance of CuGaTe2.*Appl. Phys. Lett.* 2013, **103**, 011905.
84. Li, Y. L.; Zhang, T. S.; Qin, Y. T.; Day, T.; Snyder, G. J.; Shi, X.; Chen, L. D. Thermoelectric transport properties of diamond-like Cu1−*x*Fe1+*x*S2 tetrahedral compounds. *J. Appl. Phys.* 2014, **116**, 203705.
85. Zhu, Y. C.; Liu, Y.; Wood, M.; Koocher, N. Z.; Liu, Y. Y.; Liu, L. J.; Hu, T. D.; Rondinelli, J. M.; Hong, J. W.; Snyder, G. J.; Xu, W. Synergistically Optimizing Carrier Concentration and Decreasing Sound Velocity in n-type AgInSe2 Thermoelectrics. *Chem. Mater.* 2019, **31**, 8182-8190.
86. Yan, Y.; Lu, X.; Wang, G. Y.; Zhou, X. Y. zT = 1.1 in CuInTe2 Solid Solutions Enabled by Rational Defect Engineering. *ACS Appl. Energy Mater.* 2020, **3**, 2039-2048.
87. Cao, Y.; Su, X. L.; Meng, F. C.; Bailey, T. P.; Zhao, J. G.; Xie, H. Y.; He, J.; Uher, C.; Tang, X. F. Origin of the Distinct Thermoelectric Transport Properties of Chalcopyrite ABTe2 (A = Cu, Ag; B = Ga, In). *Adv. Funct. Mater.* 2020, **30**, 2005861.
88. Song, Q. F.; Qiu, P. F.; Hao, F.; Zhao, K. P.; Zhang,T. S.; Ren, D. D.; Shi, X.; Chen, L. D. Quaternary Pseudocubic Cu2TMSnSe4 (TM = Mn, Fe, Co) Chalcopyrite Thermoelectric Materials. *Adv. Electron. Mater.* 2016, **2**, 1600312.
89. Xie, H. Y.; Su, X. L.; Zheng, G.; Zhu, T.; Yin, K.; Yan, Y. G.; Uher, C.; Kanatzidis, M. G.; Tang, X. F. The Role of Zn in Chalcopyrite CuFeS2: Enhanced Thermoelectric Properties of Cu1-*x*Zn*x*FeS2 with in-Situ Nanoprecipitates. *Adv. Energy Mater.* 2016, **7**, 1601299.
90. Zhang, J. W.; Liu, R. H.; Cheng, N.; Zhang, Y. B.; Yang, J. H.; Uher, C.; Shi, X.; Chen, L. D.; Zhang, W. Q. High-Performance Pseudocubic Thermoelectric Materials from Non-cubic Chalcopyrite Compounds. *Adv. Mater.* 2014, **26**, 3848-3853.
91. Yang, J. F.; Chen, S. P.; Du, Z. L.; Liu, X. L.; Cui, J. L. Lattice defects and thermoelectric properties: the case of p-type CuInTe2 chalcopyrite on introduction of zinc. *Dalton Trans.* 2014, **43**, 15228-15236.
92. Wang, L.; Ying, P. Z.; Deng, Y.; Zhou, H.; Du, Z. L.; Cui, J. L. Site occupations of Zn in AgInSe2-based chalcopyrites responsible for modified structures and significantly improved thermoelectric performance. *RSC Adv.* 2014, **4**, 33897-33904.
93. Schroder, T.; Rosenthal, T.; Giesbrecht, N.; Maier, S.; Scheidt, E. W.; Scherer, W.; Snyder, G. J.; Schnicka, W.; Oeckler, O. TAGS-related indium compounds and their thermoelectric properties- the solid solution series (GeTe)*x*AgIn*y*Sb1-*y*Te2 (*x* =1-12; y =0.5 and 1). *J. Mater. Chem. A* 2014, **2**, 6384-6395.
94. Shen, J. W.; Chen, Z. W.; lin, S. Q.; Zheng, L. L.; Li, W.; Pei, Z. Y. Single parabolic band behavior in thermoelectric p-type CuGaTe2.*J. Mater. Chem. C* 2016, 4, 209-214.
95. Cui, J. L.; Sun, Z.; Du, Z. L.; Chao, Y. M. Engineering the energy gap near the valence band edge in Mn-incorporated Cu3Ga5Te9 for an enhanced thermoelectric performance. *J. Mater. Chem. C* 2016, 4, 8014-8019.
96. Cui, J. L.; Lu, Y. F.; Chen, S. P.; Liu, X. L.; Du, Z. L. Unequal bonding in Ag-CuIn3Se5-based solid solutions responsible for reduction in lattice thermal conductivity and improvement in thermoelectric performance. *RSC Adv.* 2018, **8**, 9574-9579.
97. Cui, J. L.; Cai, G. M.; Ren, W. Increased effective mass and carrier concentration responsible for the improved thermoelectric performance of the nominal compound Cu2Ga4Te7 with Sb substitution for Cu. *RSC Adv.* 2018, **8**, 21637-21643.
98. Cui, J. L.; Zhu, J. H.; Han, Z. K.; Luo, Y. Significantly improved thermal stability and thermoelectric performance of Cu-deficient Cu4-*δ*Ga4Te8 (*δ*=1.12) chalcogenide through an addition of Sb. *J. Mater. Chem. A* 2018, **6**, 12672-12681.
99. Li, M.; Luo, Y.; Hu, X. J.; Han, Z. K.; Liu, X. L.; Cui, J. L. Co-regulation of the copper vacancy concentration and point defects leading to the enhanced thermoelectric performance of Cu3In5Te9-based chalcogenides. *RSC Adv.* 2019, **9**, 31747-31752.
100. Wu, H.; Dong, Z. Phase diagram of ternary Cu-Ga-Te system and thermoelectric properties of chalcopyrite CuGaTe2 materials. *Acta Materialia* 2016, **118**, 331e341
101. Carr, W. D.; Morelli, D. T. Influence of doping and solid solution formation on the thermoelectric properties of chalcopyrite semiconductors. *J. Alloy. Compd.* 2015, **630**, 277-281.
102. Ge, B. Z.; Shi, Z. Q.; Zhou, C. J.; Hu, J. B.; Liu, G. W.; Xia, H. Y.; Xu, J. T.; Qiao, G. J. Enhanced thermoelectric performance of n-Type eco-friendly material Cu1-*x*Ag*x*FeS2 (*x*=0-0.14) via bandgap tuning. *J. Alloy. Compd.* 2019, **809**, 151717.
103. Ahmed, F.; Tsujii, N.; Mori, T. Microstructure analysis and thermoelectric properties of iron doped CuGaTe2. *[J. Materiomics](http://www.letpub.com.cn/index.php?page=journalapp&view=detail&journalid=10877)* 2018, **4**, 221-227.
104. Kucek, V.; Drasar, C.; Navratil, J.; Plechacek, T.; Benes, L.Thermoelectric properties of Ni-doped CuInTe2.*J. Phys. Chem. Solids* 2015, **83**, 18-23.
105. Ye, Z. X.; Cho, J. Y.; Tessema, M. M.; Salvador, J. R.; Waldo, R. A.; Wang, H.; Cai, W. The effect of structural vacancies on the thermoelectric properties of (Cu2Te)1-*x*(Ga2Te3)*x.J. Solid State Chem.* 2013, **201**, 262-269.
106. Luo, Y. B.; Jiang, J. H.; Yang, J. Y.; Li, W. X.; Zhang, D.; Zhou, Z. W.; Cheng, Y. D.; Ren, Y. Y.; He, X.; Li, X. Simultaneous regulation of electrical and thermal transport properties in CuInTe2 by directly incorporating excess ZnX (X=S, Se). *Nano Energy* 2017, **32**, 80-87.
107. Kumagai, M.; Kurosaki, K.; Ohishi, Y.; Muta, H.; Yamanaka, S. Effect of Ball-Milling Conditions on Thermoelectric Properties of Polycrystalline CuGaTe2. *Mater. Trans.* 2014, **55**, 1215-1218.
108. Li, W. X.; Luo, Y. B.; Zheng, Y.; Du, C. F.; Liang, Q. H.; Zhu, B. B.; Zhao, L. Enhancement of the thermoelectric performance of CuInTe2 via SnO2 in-situ replacement. *J. Mater. Sci-Mater. El.* 2018, **29**, 4732-4737.
109. Li, J.; Zhang, X.; Chen, Z.; Lin, S.; Li, W.; Shen, J.; Witting, I. T.; Faghaninia, A.; Chen, Y.; Jain, A.; et al. Low-Symmetry Rhombohedral GeTe Thermoelectrics. *Joule* 2018, **2**, 976-987.
110. Wu, D.; Xie, L.; Xu, X.; He, J. High Thermoelectric Performance Achieved in GeTe-Bi2Te3 Pseudo-Binary via Van der Waals GapInduced Hierarchical Ferroelectric Domain Structure. *Adv. Funct. Mater.* 2019, **29**, 1806613.
111. Xu, X.; Xie, L.; Lou, Q.; Wu, D.; He, J. Boosting the Thermoelectric Performance of Pseudo-Layered Sb2Te3(GeTe)*n* via Vacancy Engineering. *Adv. Sci.* 2018, **5**, 1801514.
112. Bayikadi, K. s.; Wu, C. T.; Chen, L.-C.; Chen, K. H.; Chou, F.-C.; Sankar, R. Synergistic Optimization of Thermoelectric Performance of Sb Doped GeTe with Strained Domain and Domain Boundaries. *J. Mater. Chem. A* 2020, **8**, 5332-5341.
113. Hong, M.; Chen, Z.-G.; Yang, L.; Zou, Y.-C.; Dargusch, M. S.; Wang, H.; Zou, J. Realizing zT of 2.3 in Ge1‑*x*‑*y*Sb*x*In*y*Te via Reducing the Phase-Transition Temperature and Introducing Resonant Energy Doping. *Adv. Mater.* 2018, **30**, 1705942.
114. Zhang, X.; Li, J.; Wang, X.; Chen, Z.; Mao, J.; Chen, Y.; Pei, Y. Vacancy Manipulation for Thermoelectric Enhancements in GeTe Alloys. *J. Am. Chem. Soc.* 2018, **140**, 15883-15888.
115. Gelbstein, Y.; Davidow, J.; Girard, S. N.; Chung, D. Y.; Kanatzidis, M. Controlling Metallurgical Phase Separation Reactions of the Ge0.87Pb0.13Te Alloy for High Thermoelectric Performance. *Adv. Energy Mater.* 2013, **3**, 815-820.
116. Koenig, J.; Winkler, M.; Dankwort, T.; Hansen, A.-L.; Pernau, H.- F.; Duppel, V.; Jaegle, M.; Bartholome, K.; Kienle, L.; Bensch, W. Thermoelectric Efficiency of (1-*x*)(GeTe)*x*(Bi2Se0.2Te2.8) and Implementation into Highly Performing Thermoelectric Power Generators. *Dalton T.* 2015, **44**, 2835-2843.
117. Lou, Q.; Xu, X.; Huang, Y.; Zhu, B.; Yu, Y.; He, J. Excellent Thermoelectric Performance Realized in p-Type Pseudolayered Sb2Te3(GeTe)12 via Rhenium Doping. *ACS Appl. Energy Mater.* 2020, **3**, 2063-2069.
118. Li, J.; Chen, Z.; Zhang, X.; Yu, H.; Wu, Z.; Xie, H.; Chen, Y.; Pei, Y. Simultaneous Optimization of Carrier Concentration and Aloy Scattering for Ultrahigh Performance GeTe Thermoelectrics. *Adv. Sci.* 2017, **4**, 1700341.
119. Hong, M.; Zheng, K.; Lyv, W.; Li, M.; Qu, X.; Sun, Q.; Xu, S.; Zou, J.; Chen, Z.-G. Computer-Aided Design of High-Efficiency GeTeBased Thermoelectric Devices. *Energy Environ. Sci.* 2020, **13**, 1856.
120. Hong, M.; Wang, Y.; Liu, W.; Matsumura, S.; Wang, H.; Zou, J.; Chen, Z. G. Arrays of Planar Vacancies in Superior Thermoelectric Ge1‑*x*‑*y*Cd*x*Bi*y*Te with Band Convergence. *Adv. Energy Mater.* 2018, **8**, 1801837.
121. Wu, D.; Xie, L.; Chao, X.; Yang, Z.; He, J. Step-Up Thermoelectric Performance Realized in Bi2Te3 Alloyed GeTe via Carrier Concentration and Microstructure Modulations. *ACS Appl. Energy Mater.* 2019, **2**, 1616-1622.
122. Xu, X.; Huang, Y.; Xie, L.; Wu, D.; Ge, Z.; He, J. Realizing Improved Thermoelectric Performance in BiI3-Doped Sb2Te3(GeTe)17 via Introducing Dual Vacancy Defects. *Chem. Mater.* 2020, **32**, 1693-1701.
123. Li, M.; Hong, M.; Tang, X.; Sun, Q.; Lyu, W.-Y.; Xu, S.-D.; Kou, L.-Z.; Dargusch, M.; Zou, J.; Chen, Z.-G. Crystal Symmetry Induced Structure and Bonding Manipulation Boosting Thermoelectric Performance of GeTe. *Nano Energy* 2020, **73**, 104740.
124. Samanta, M.; Biswas, K. Low Thermal Conductivity and High Thermoelectric Performance in (GeTe)1‑2*x*(GeSe)*x*(GeS)*x*: Competition between Solid Solution and Phase Separation. *J. Am. Chem. Soc.* 2017, **139**, 9382-9391.
125. Perumal, S.; Samanta, M.; Ghosh, T.; Shenoy, U. S.; Bohra, A. K.; Bhattacharya, S.; Singh, A.; Waghmare, U. V.; Biswas, K. Realization of High Thermoelectric Figure of Merit in GeTe by Complementary Co-doping of Bi and In. *Joule* 2019, **3**, 2565-2580.
126. Jin, Y.; Zhang, X.; Xiao, Y.; He, W.; Wang, D.; Li, J.; Zheng, S.; Ren, D.; Qiu, Y.; Zhao, L.-D. Synergistically Improving Thermoelectric and Mechanical Properties of Ge0.94Bi0.06Te through Dispersing NanoSiC. *Scr. Mater.* 2020, **183**, 22-27.
127. Qiu, Y.; Jin, Y.; Wang, D.; Guan, M.; He, W.; Peng, S.; Liu, R.; Gao, X.; Zhao, L.-D. Realizing High Thermoelectric Performance in GeTe through Decreasing the Phase Transition Temperature via Entropy Engineering. *J. Mater. Chem. A* 2019, **7**, 26393-26401.
128. Xie, L.; Chen, Y.; Liu, R.; Song, E.; Xing, T.; Deng, T.; Song, Q.; Liu, J.; Zheng, R.; Gao, X.; et al. Stacking Faults Modulation for Scattering Optimization in GeTe-Based Thermoelectric Materials. *Nano Energy* 2020, **68**, 104347.
129. Li, J.; Xie, Y.; Zhang, C.; Ma, K.; Liu, F.; Ao, W.; Li, Y.; Zhang, C. Stacking Fault-Induced Minimized Lattice Thermal Conductivity in the High-Performance GeTe-Based Thermoelectric Materials upon Bi2Te3 Alloying. *ACS Appl. Mater. Interfaces* 2019, **11**, 20064-20072.
130. Shuai, J.; Sun, Y.; Tan, X.; Mori, T. Manipulating the Ge Vacancies and Ge Precipitates through Cr Doping for Realizing the High-Performance GeTe Thermoelectric Material. *Small* 2020, **16**, 1906921.
131. Li, J.; Zhang, X.; Lin, S.; Chen, Z.; Pei, Y. Realizing the High Thermoelectric Performance of GeTe by Sb-Doping and Se-Alloying. *Chem. Mater.* 2017, **29**, 605-611.
132. Dong, J.; Sun, F.-H.; Tang, H.; Pei, J.; Zhuang, H.-L.; Hu, H.-H.; Zhang, B.-P.; Pan, Y.; Li, J.-F. Medium-Temperature Thermoelectric GeTe: Vacancy Suppression and Band Structure Engineering Leading to High Performance. *Energy Environ. Sci.* 2019, **12**, 1396-1403.
133. Srinivasan, B.; Gelle, A.; Gucci, F.; Boussard-Pledel, C.; Fontaine, B.; Gautier, R.; Halet, J.-F.; Reece, M. J.; Bureau, B. Realizing a Stable High Thermoelectric zT~ 2 over a Broad Temperature Range in Ge1‑*x*‑*y*Ga*x*Sb*y*Te via Band Engineering and Hybrid Flash-SPS Processing. *Inorg. Chem. Front.* 2019, **6**, 63-73.
134. Li, P.; Ding, T.; Li, J.; Zhang, C.; Dou, Y.; Li, Y.; Hu, L.; Liu, F.; Zhang, C. Positive Effect of Ge Vacancies on Facilitating Band Convergence and Suppressing Bipolar Transport in GeTe-Based Alloys for High Thermoelectric Performance. *Adv. Funct. Mater.* 2020, **30**, 1910059.
135. Wang, L.; Li, J.; Zhang, C.; Ding, T.; Xie, Y.; Li, Y.; Liu, F.; Ao, W.; Zhang, C. Discovery of Low-Temperature GeTe-Based Thermoelectric Alloys with High Performance Competing with Bi2Te3. *J. Mater. Chem. A* 2020, **8**, 1660-1667.
136. Jin, Y.; Xiao, Y.; Wang, D.; Huang, Z.; Qiu, Y.; Zhao, L.-D. Realizing High Thermoelectric Performance in GeTe through Optimizing Ge Vacancies and Manipulating Ge Precipitates. *ACS Appl. Energy Mater.* 2019, **2**, 7594-7601.
137. Wei, P.-C.; Cai, C.-X.; Hsing, C.-R.; Wei, C.-M.; Yu, S.-H.; Wu, H.-J.; Chen, C.-L.; Wei, D.-H.; Nguyen, D.-L.; Chou, M. M. C.; Chen, Y.-Y. Enhancing Thermoelectric Performance by Fermi Level Tuning and Thermal Conductivity Degradation in (Ge1‑*x*Bi*x*)Te Crystals. *Sci. Rep.* 2019, **9**, 8616.
138. Tan, H.; Zhang, B.; Wang, G.; Chen, Y.; Shen, X.; Guo, L.; Han, X.; Lu, X.; Zhou, X. Rapid Preparation of Ge0.9Sb0.1Te1+*x* via Unique Melt Spinning: Hierarchical Microstructure and Improved Thermoelectric Performance. *J. Alloys Compd.* 2019, **774**, 129-136.
139. Perumal, S.; Roychowdhury, S.; Negi, D. S.; Datta, R.; Biswas, K. High Thermoelectric Performance and Enhanced Mechanical Stability of p-Type Ge1‑*x*Sb*x*Te. *Chem. Mater.* 2015, **27**, 7171-7178.
140. Xing, T.; Song, Q.; Qiu, P.; Zhang, Q.; Xia, X.; Liao, J.; Liu, R.; Huang, H.; Yang, J.; Bai, S.; et al. Superior Performance and High Service Stability for GeTe-Based Thermoelectric Compounds. *Natl. Sci. Rev.* 2019, **6**, 944-954.
141. Perumal, S.; Bellare, P.; Shenoy, U. S.; Waghmare, U. V.; Biswas, K. Low Thermal Conductivity and High Thermoelectric Performance in Sb and Bi Codoped GeTe: Complementary Effect of Band Convergence and Nanostructuring. *Chem. Mater.* 2017, **29**, 10426-10435.
142. Nshimyimana, E.; Hao, S.; Su, X.; Zhang, C.; Liu, W.; Yan, Y.; Uher, C.; Wolverton, C.; Kanatzidis, M. G.; Tang, X. Discordant Nature of Cd in GeTe Enhances Phonon Scattering and Improves Band Convergence for High Thermoelectric Performance. *J. Mater. Chem. A* 2020, **8**, 1193-1204.
143. Liu, H.; Zhang, X.; Li, J.; Bu, Z.; Meng, X.; Ang, R.; Li, W. Band and Phonon Engineering for Thermoelectric Enhancements of Rhombohedral GeTe. *ACS Appl. Mater. Interfaces* 2019, **11**, 30756-30762.
144. [Kim, H. S](http://apps.webofknowledge.com/OutboundService.do?SID=5FJ3zU4jD3OkweO9UcE&mode=rrcAuthorRecordService&action=go&product=WOS&lang=zh_CN&daisIds=1632887" \o "查找此作者的更多记录).; [Madavali, B](http://apps.webofknowledge.com/OutboundService.do?SID=5FJ3zU4jD3OkweO9UcE&mode=rrcAuthorRecordService&action=go&product=WOS&lang=zh_CN&daisIds=2477048" \o "查找此作者的更多记录).; [Hong, S. J](http://apps.webofknowledge.com/OutboundService.do?SID=5FJ3zU4jD3OkweO9UcE&mode=rrcAuthorRecordService&action=go&product=WOS&lang=zh_CN&daisIds=159157" \o "查找此作者的更多记录).; [Kim, T. S](http://apps.webofknowledge.com/OutboundService.do?SID=5FJ3zU4jD3OkweO9UcE&mode=rrcAuthorRecordService&action=go&product=WOS&lang=zh_CN&daisIds=60734" \o "查找此作者的更多记录). Effect of Milling Time on the Microstructure and Thermoelectric Properties of p-Type TAGS-90 Alloys by HEM and SPS. *Int. J. Appl. Ceram. Technol.* 2016, **13**, 239-244.
145. Zhu, T.; Gao, H.; Chen, Y.; Zhao, X. Ioffe-Regel Limit and Lattice Thermal Conductivity Reduction of High Performance (AgSbTe2)15(GeTe)85 Thermoelectric Materials. *J. Mater. Chem. A* 2014, **2**, 3251-3256.
146. Hazan, E.; Madar, N.; Parag, M.; Casian, V.; Ben-Yehuda, O.; Gelbstein, Y. Effective Electronic Mechanisms for Optimizing the Thermoelectric Properties of GeTe-Rich Alloys. *Adv. Electron. Mater.* 2015, **1**, 1500228.
147. Zhang, L.; Wang, W.; Ren, B.; Yan, Y. Thermoelectric Performance and High-Temperature Creep Behavior of GeTe-Based Thermoelectric Materials. *J. Electron. Mater.* 2011, **40**, 1057-1061.
148. Gelbstein, Y. Phase Morphology Effects on the Thermoelectric Properties of Pb0.25Sn0.25Ge0.5Te. *Acta Mater.* 2013, **61**, 1499-1507.
149. Mohanraman, R.; Sankar, R.; Chou, F. C.; Lee, C. H.; Chen, Y. Y. Enhanced thermoelectric performance in Bi-doped p-type AgSbTe2 compounds. *J. Appl. Phys.* 2013, **114**, 163712.
150. Wu, H. J.; Lan, T. W.; Chen, S. W.; Chen, Y. Y.; Day, T.; Snyder, G. J. State of the art Ag50-*x*Sb*x*Se50-*y*Te*y* alloys: Their high zT values, microstructures and related phase equilibria. *Acta Materialia* 2015, **93**, 38-45.
151. Zhang, H.; Luo, J.; Zhu, H. T.; Liu, Q. L.; Liang, J. K.; Li, J. B.; Liu, G. Y. Synthesis and thermoelectric properties of Mn-doped AgSbTe2 compounds. *Chin. Phys. B* 2012, **21**, 106101.
152. Li, K.; Li, Z.; Yang, L.; Xiao, C.; Xie, Y. Charge Compensation Modulation of the Thermoelectric Properties in AgSbTe2 via Mn Amphoteric Doping. *Inorg. Chem.* 2019, **58**, 9205-9212.
153. Roychowdhury, S.; Panigrahi, R.; Perumal, S.; Biswas, K. Ultrahigh Thermoelectric Figure of Merit and Enhanced Mechanical Stability of p‑type AgSb1-*x*Zn*x*Te2. *ACS Energy Lett.* 2017, **2**, 349-356.
154. Tan, G. J.; Hao, S. Q.; Hanus, R. C.; Zhang, X. M.; Anand, S.; Bailey, T. P.; Rettie, A. J. E.; Su, X. L.; Uher, C.; Dravid, V. P.; Snyder, G. J.; Wolverton, C.; Kanatzidis, M. G. High Thermoelectric Performance in SnTe-AgSbTe2 Alloys from Lattice Softening, Giant Phonon-Vacancy Scattering, and Valence Band Convergence. *ACS Energy Lett.* 2018, **3**, 705-712.
155. Mohanraman, R.; Sankar, R.; Chou, F. C.; Lee, C. H.; Lizuka，Y.; Muthuselvam, I. P.; Chen, Y. Y. Inflfluence of nanoscale Ag2Te precipitates on the thermoelectric properties of the Sn doped p-Type AgSbTe2 compound. *APL Mater.* 2014, **2**, 096114.
156. Chen, Y.; Nielsen, M. D.; Gao, Y. B.; Zhu, T. J.; Zhao, X. B.; Heremans, J. P. SnTe-AgSbTe2 Thermoelectric Alloys. *Adv. Energy Mater.* 2012, **2**, 58-62.
157. Han, M. K.; Androulakis, J.; Kim, S. J.; Kanatzidis, M. G. Lead-Free Thermoelectrics: High Figure of Merit in p-type AgSn*m*SbTe*m*+2. *Adv. Energy Mater.* 2012, **2**, 157-161.
158. Hong, M.; Chen, Z. G.; Yang, L.; Liao, Z. M.; Zou, Y. C.; Chen, Y. H.; Matsumura, S.; Zou, J. Achieving zT > 2 in p-Type AgSbTe2-*x*Se*x* Alloys via Exploring the Extra Light Valence Band and Introducing Dense Stacking Faults. *Adv. Energy Mater.* 2018, **8**, 1702333.
159. Xu, J. J.; Li, H.; Du, B. L.; Tang, X. F.; Zhang, Q. J.; Uher, C. High thermoelectric figure of merit and nanostructuring in bulk AgSbTe2. *J. Mater. Chem.* 2010, **20**, 6138-6143.
160. Guin, S. N.; Chatterjee, A.; Negi, D. S.; Datta, R.; Biswas, K. High Thermoelectric Performance in Tellurium Free p-type AgSbSe2. *Energy Environ. Sci.* 2013, **6**, 2603-2608.
161. Mohanraman, R.; Sankar, R.; Boopathi, K. M.; Chou, F. C.; Chu, C. W.; Lee, C. H.; Chen, Y. Y. Influence of In doping on the thermoelectric properties of an AgSbTe2 compound with enhanced figure of merit. *J. Mater. Chem. A* 2014, **2**, 2839-2844.
162. Guin, S. N.; Negi, D. S.; Datta, R.; Biswas, K. Nanostructuring, carrier engineering and bond anharmonicity synergistically boost the thermoelectric performance of p-type AgSbSe2-ZnSe. *J. Mater. Chem. A* 2014, **2**, 4324-4331.
163. Guin, S. N.; Chatterjee, A.; Biswas, K. Enhanced thermoelectric performance in p-type AgSbSe2 by Cd-doping. R*SC Adv.* 2014, **4**, 11811-11815.
164. Guin, S. N.; Biswas, K. Sb deficiencies control hole transport and boost the thermoelectric performance of p-type AgSbSe2. *J. Mater. Chem. C* 2015, **3**, 10415-10421.
165. Du, B. L.; Li, H.; Xu, J. J.; Tang, X. F.; Uher, C. Enhanced Figure-of-Merit in Se-Doped p-Type AgSbTe2 Thermoelectric Compound. *Chem. Mater.* 2010, **22**, 5521-5527.
166. Du, B. L.; Li, H.; Tang, X. F. Enhanced thermoelectric performance in Na-doped p-type nonstoichiometric AgSbTe2 compound. *J. Alloy. Compd.* 2011, **509**, 2039-2043.
167. Pan, L.; Berardan, D.; Dragoe, N. High Thermoelectric Properties of n‑Type AgBiSe2. *J. Am. Chem. Soc.* 2013, **135**, 4914-4917.
168. Min, B. K.; Kin, B. S.; Oh, M. W.; Ryu, B. K.; Lee, J. E.; Joo, S. J.; Park, S. D.; Lee, H. W. Effect of La-doping on AgSbTe2 Thermoelectric Compounds. *J. Korean Phys. Soc.* 2016, **68**, 164-169.
169. Yusufu, A.; Kurosaki, K.; Muta, H.; Yamanaka, S. Effect of (Pb,Ge)Te addition on the phase stability and the thermoelectric properties of AgSbTe2. *Mater. Res. Soc. Symp. Proc.* 2010, **1267**.
170. Du, B.; Xu, J.; Zhang, W.; Tang, X. Impact of *In Situ* Generated Ag2Te Nanoparticles on the Microstructure and Thermoelectric Properties of AgSbTe2 Compounds. *J. Electron. Mater.* 2011, **40**, 1249-1253.
171. Du, B.; Li, H.; Tang, X. Effect of Ce Substitution for Sb on the Thermoelectric Properties of AgSbTe2 Compound. *J. Electron. Mater.* 2014, **43**, 2384-2389.
172. Zhang, J.; Qin, X. Y.; Li, D.; Song, C. J.; Liu, Y. F.; Xin, H. X.; Zou, T. H.; Li, Y. Y. Optimized Thermoelectric Properties of AgSbTe2 through Adjustment of Fabrication Parameters. *Electron. Mater. Lett.* 2015, **11**, 133-137.
173. Shi, X.; Yang, J.; Salvador, J. R.; Chi, M.; Cho, J. Y.; Wang, H.; Bai, S.; Yang, J.; Zhang, W.; Chen, L. Multiple-Filled Skutterudites: High Thermoelectric Figure of Merit through Separately Optimizing Electrical and Thermal Transports. *J. Am. Chem. Soc.* 2011, **133**, 7837-7846.
174. Guo, J.; Geng, H.; Ochi, T.; Suzuki, S.; Kikuchi, M.; Yamaguchi, Y.; Ito, S. Development of Skutterudite Thermoelectric Materials and Modules. *J. Electron. Mater.* 2012, **41**, 1036-1042.
175. Zhou, X.; Wang, G.; Zhang, L.; Chi, H.; Su, X.; Sakamoto, J.; Uher, C. Enhanced Thermoelectric Properties of Ba-Filled Skutterudites by Grain Size Reduction and Ag Nanoparticle Inclusion. *J. Mater. Chem.* 2012, **22**, 2958-2964.
176. Ballikaya, S.; Uzar, N.; Yildirim, S.; Salvador, J. R.; Uher, C. High Thermoelectric Performance of In, Yb, Ce Multiple Filled CoSb3 Based Skutterudite Compounds. *J. Solid State Chem.* 2012, **193**, 31-35.
177. Tang, Y.; Gibbs, Z. M.; Agapito, L. A.; Li, G.; Kim, H. S.; Nardelli, M. B.; Curtarolo, S.; Snyder, G. J. Convergence of Multi Valley Bands as the Electronic Origin of High Thermoelectric Performance in CoSb3 Skutterudites. *Nat. Mater.* 2015, **14**, 1223-1228.
178. Tang, Y.; Qiu, Y.; Xi, L.; Shi, X.; Zhang, W.; Chen, L.; Tseng, S. M.; Chen, S.W.; Snyder, G. J. Phase Diagram of In-Co-Sb System and Thermoelectric Properties of In-Containing Skutterudites. *Energy Environ. Sci.* 2014, **7**, 812-819.
179. Zhou, X.; Wang, G.; Guo, L.; Chi, H.; Wang, G.; Zhang, Q.; Chen, C.; Thompson, T.; Sakamoto, J.; Dravid, V. P.; et al. Hierarchically Structured TiO2 for Ba-Filled Skutterudite with Enhanced Thermoelectric Performance. *J. Mater. Chem. A* 2014, **2**, 20629-20635.
180. Ballikaya, S.; Uher, C. Enhanced Thermoelectric Performance of Optimized Ba, Yb Filled and Fe Substituted Skutterudite Compounds. *J. Alloys Compd.* 2014, **585**, 168-172.
181. Rogl, G.; Grytsiv, A.; Yubuta, K.; Puchegger, S.; Bauer, E.; Raju, C.; Mallik, R.; Rogl, P. In-Doped Multifilled n-Type Skutterudites with ZT = 1.8. *Acta Mater.* 2015, **95**, 201-211.
182. Zong, P. A.; Hanus, R.; Dylla, M.; Tang, Y.; Liao, J.; Zhang, Q.; Snyder, G. J.; Chen, L. Skutterudite with Graphene-Modified GrainBoundary Complexion Enhances zT Enabling High-Efficiency Thermoelectric Device. *Energy Environ. Sci.* 2017, **10**, 183-191.
183. Meng, X.; Liu, Z.; Cui, B.; Qin, D.; Geng, H.; Cai, W.; Fu, L.; He, J.; Ren, Z.; Sui, J. Grain Boundary Engineering for Achieving High Thermoelectric Performance in n-Type Skutterudites. *Adv. Energy Mater.* 2017, **7**, 1602582.
184. Zhang, Q.; Zhou, Z.; Dylla, M.; Agne, M. T.; Pei, Y.; Wang, L.; Tang, Y.; Liao, J.; Li, J.; Bai, S.; et al. Realizing High-Performance Thermoelectric Power Generation through Grain Boundary Engineering of Skutterudite-Based Nanocomposites. *Nano Energy* 2017, **41**, 501-510.
185. Rogl, G.; Bursik, J.; Grytsiv, A.; Puchegger, S.; Soprunyuk, V.; Schranz, W.; Yan, X.; Bauer, E.; Rogl, P. Nanostructuring as a Tool to Adjust Thermal Expansion in High ZT Skutterudites. *Acta Mater.* 2018, **145**, 359-368.
186. Lee, S.; Lee, K. H.; Kim, Y.-M.; Kim, H. S.; Snyder, G. J.; Baik, S.; Kim, S. W. Simple and Efficient Synthesis of Nanograin Structured Single Phase Filled Skutterudite for High Thermoelectric Performance. *Acta Mater.* 2018, **142**, 8-17.
187. Zhou, Z.; Li, J.; Fan, Y.; Zhang, Q.; Lu, X.; Fan, S.; Kikuchi, K.; Nomura, N.; Kawasaki, A.; Wang, L.; Jiang, W. Uniform Dispersion of SiC in Yb-Filled Skutterudite Nanocomposites with High Thermoelectric and Mechanical Performance. *Scr. Mater.* 2019, **162**, 166-171.
188. Qin, D.; Cui, B.; Meng, X.; Qin, P.; Xie, L.; Zhang, Q.; Liu, W.; Cao, J.; Cai, W.; Sui, J. High Thermoelectric Performance from High Carrier Mobility and Reduced Lattice Thermal Conductivity in Ba, Yb Double-Filled Skutterudites. *Mater. Today Phys.* 2019, **8**, 128-137.
189. Nie, G.; Li, W.; Guo, J.; Yamamoto, A.; Kimura, K.; Zhang, X.; Isaacs, E. B.; Dravid, V.; Wolverton, C.; Kanatzidis, M. G.; et al. High Performance Thermoelectric Module through Isotype Bulk Heterojunction Engineering of Skutterudite Materials. *Nano Energy* 2019, **66**, 104193.
190. Li, W.; Wang, J.; Xie, Y.; Gray, J. L.; Heremans, J. J.; Kang, H. B.; Poudel, B.; Huxtable, S. T.; Priya, S. Enhanced Thermoelectric Performance of Yb-Single-Filled Skutterudite by Ultralow Thermal Conductivity. *Chem. Mater.* 2019, **31**, 862-872.
191. Qin, D.; Cui, B.; Yin, L.; Zhao, X.; Zhang, Q.; Cao, J.; Cai, W.; Sui, J. Tin Acceptor Doping Enhanced Thermoelectric Performance of n-Type Yb Single-Filled Skutterudites via Reduced Electronic Thermal Conductivity. *ACS Appl. Mater. Interfaces* 2019, **11**, 25133-25139.
192. Zhao, W.; Liu, Z.; Sun, Z.; Zhang, Q.; Wei, P.; Mu, X.; Zhou, H.; Li, C.; Ma, S.; He, D.; et al. Superparamagnetic Enhancement of Thermoelectric Performance. *Nature* 2017, **549**, 247-251.
193. Zhao, W.; Liu, Z.; Wei, P.; Zhang, Q.; Zhu, W.; Su, X.; Tang, X.; Yang, J.; Liu, Y.; Shi, J.; et al. Magnetoelectric Interaction and Transport Behaviours in Magnetic Nanocomposite Thermoelectric Materials. *Nat. Nanotechnol.* 2017, **12**, 55.
194. Chauhan, N. S.; Bathula, S.; Vishwakarma, A.; Bhardwaj, R.; Johari, K. K.; Gahtori, B.; Saravanan, M.; Dhar, A. Compositional Tuning of ZrNiSn Half-Heusler Alloys: Thermoelectric Characteristics and Performance Analysis. *J. Phys. Chem. Solids* 2018, **123**, 105-112.
195. Gurth, M.; Rogl, G.; Romaka, V.; Grytsiv, A.; Bauer, E.; Rogl, P. Thermoelectric High ZT Half-Heusler Alloys Ti1‑*x*‑*y*Zr*x*Hf*y*NiSn (0≤*x*≤1; 0≤*y*≤1). *Acta Mater.* 2016, **104**, 210-222.
196. Zhang, H.; Wang, Y.; Dahal, K.; Mao, J.; Huang, L.; Zhang, Q.; Ren, Z. Thermoelectric Properties of n-Type Half-Heusler Compounds (Hf0.25Zr0.75)1‑*x*Nb*x*NiSn. *Acta Mater.* 2016, **113**, 41-47.
197. Populoh, S.; Aguirre, M.; Brunko, O.; Galazka, K.; Lu, Y.; Weidenkaff, A. High Figure of Merit in (Ti,Zr,Hf)NiSn Half-Heusler Alloys. *Scr. Mater.* 2012, **66**, 1073-1076.
198. Shen, J.; Fu, C.; Liu, Y.; Zhao, X.; Zhu, T. Enhancing Thermoelectric Performance of FeNbSb Half-Heusler Compound by Hf-Ti Dual-Doping. *Energy Storage Mater.* 2018, **10**, 69-74.
199. Rausch, E.; Balke, B.; Ouardi, S.; Felser, C. Enhanced Thermoelectric Performance in the p-Type Half-Heusler (Ti/Zr/Hf)CoSb0.8Sn0.2 System via Phase Separation. *Phys. Chem. Chem. Phys.* 2014, **16**, 25258-25262.
200. Fu, C.; Zhu, T.; Liu, Y.; Xie, H.; Zhao, X. Band Engineering of High Performance p-Type FeNbSb Based Half-Heusler Thermoelectric Materials for Figure of Merit ZT > 1. *Energy Environ. Sci.* 2015, **8**, 216-220.
201. Rausch, E.; Balke, B.; Stahlhofen, J. M.; Ouardi, S.; Burkhardt, U.; Felser, C. Fine Tuning of Thermoelectric Performance in PhaseSeparated Half-Heusler Compounds. *J. Mater. Chem. C* 2015, **3**, 10409-10414.
202. Chen, S.; Lukas, K. C.; Liu, W.; Opeil, C. P.; Chen, G.; Ren, Z. Effect of Hf Concentration on Thermoelectric Properties of Nano-structured n-Type Half-Heusler Materials HfxZr1‑*x*NiSn0.99Sb0.01. *Adv. Energy Mater.* 2013, **3**, 1210-1214.
203. Poon, S. J.; Wu, D.; Zhu, S.; Xie, W.; Tritt, T. M.; Thomas, P.; Venkatasubramanian, R. Half-Heusler Phases and Nanocomposites as Emerging High-ZT Thermoelectric Materials. *J. Mater. Res.* 2011, **26**, 2795-2802.
204. Joshi, G.; Yan, X.; Wang, H.; Liu, W.; Chen, G.; Ren, Z. Enhancement in Thermoelectric Figure-of-Merit of an n-Type HalfHeusler Compound by the Nanocomposite Approach. *Adv. Energy Mater.* 2011, **1**, 643-647.
205. Fu, C.; Bai, S.; Liu, Y.; Tang, Y.; Chen, L.; Zhao, X.; Zhu, T. Realizing High Figure of Merit in Heavy-Band p-Type Half-Heusler Thermoelectric Materials. *Nat. Commun.* 2015, **6**, 8144.
206. Yan, X.; Joshi, G.; Liu, W.; Lan, Y.; Wang, H.; Lee, S.; Simonson, J.; Poon, S.; Tritt, T.; Chen, G.; Ren, Z. F. Enhanced Thermoelectric Figure of Merit of p-Type Half-Heuslers. *Nano Lett.* 2011, **11**, 556-560.
207. Zhu, H.; He, R.; Mao, J.; Zhu, Q.; Li, C.; Sun, J.; Ren, W.; Wang, Y.; Liu, Z.; Tang, Z.; et al. Discovery of ZrCoBi Based Half Heuslers with High Thermoelectric Conversion Efficiency. *Nat. Commun.* 2018, **9**, 2497.
208. Xie, H.; Wang, H.; Pei, Y.; Fu, C.; Liu, X.; Snyder, G. J.; Zhao, X.; Zhu, T. Beneficial Contribution of Alloy Disorder to Electron and Phonon Transport in Half-Heusler Thermoelectric Materials. *Adv. Funct. Mater.* 2013, **23**, 5123-5130.
209. Yu, J.; Fu, C.; Liu, Y.; Xia, K.; Aydemir, U.; Chasapis, T. C.; Snyder, G. J.; Zhao, X.; Zhu, T. Unique Role of Refractory Ta Alloying in Enhancing the Figure of Merit of NbFeSb Thermoelectric Materials. *Adv. Energy Mater.* 2018, **8**, 1701313.
210. Liu, Z.; Guo, S.; Wu, Y.; Mao, J.; Zhu, Q.; Zhu, H.; Pei, Y.; Sui, J.; Zhang, Y.; Ren, Z. Design of High-Performance Disordered HalfHeusler Thermoelectric Materials Using 18-Electron Rule. *Adv. Funct. Mater.* 2019, **29**, 1905044.
211. Qiu, Q.; Liu, Y.; Xia, K.; Fang, T.; Yu, J.; Zhao, X.; Zhu, T. Grain Boundary Scattering of Charge Transport in n-Type (Hf,Zr)CoSb HalfHeusler Thermoelectric Materials. *Adv. Energy Mater.* 2019, **9**, 1803447.
212. Farooq, M.; Butt, S.; Gao, K.; Zhu, Y.; Sun, X.; Pang, X.; Khan, S. U.; Mohmed, F.; Mahmood, A.; Mahmood, N.; Xu, W. Cd-Doping a Facile Approach for Better Thermoelectric Transport Properties of BiCuSeO Oxyselenides. *RSC Adv.* 2016, **6**, 33789-33797.
213. Lan, J. L.; Liu, Y. C.; Zhan, B.; Lin, Y. H.; Zhang, B.; Yuan, X.; Zhang, W.; Xu, W.; Nan, C. W. Enhanced Thermoelectric Properties of Pb-Doped BiCuSeO Ceramics. *Adv. Mater.* 2013, **25**, 5086-5090.
214. Li, F.; Wei, T.-R.; Kang, F.; Li, J.-F. Enhanced Thermoelectric Performance of Ca-Doped BiCuSeO in a Wide Temperature Range. *J. Mater. Chem. A* 2013, **1**, 11942-11949.
215. Li, J.; Sui, J.; Pei, Y.; Meng, X.; Berardan, D.; Dragoe, N.; Cai, W.; Zhao, L.-D. The Roles of Na Doping in BiCuSeO Oxyselenides as a Thermoelectric Material. J*. Mater. Chem. A* 2014, **2**, 4903-4906.
216. Li, J.; Sui, J.; Pei, Y.; Barreteau, C.; Berardan, D.; Dragoe, N.; Cai, W.; He, J.; Zhao, L.-D. A High Thermoelectric Figure of Merit ZT > 1 in Ba Heavily Doped BiCuSeO Oxyselenides. *Energy Environ. Sci.* 2012, **5**, 8543-8547.
217. Liu, Y.; Zhao, L.-D.; Liu, Y.; Lan, J.; Xu, W.; Li, F.; Zhang, B.-P.; Berardan, D.; Dragoe, N.; Lin, Y.-H.; et al. Remarkable Enhancement in Thermoelectric Performance of BiCuSeO by Cu Deficiencies. *J. Am. Chem. Soc.* 2011, **133**, 20112-20115.
218. Pei, Y.-L.; He, J.; Li, J.-F.; Li, F.; Liu, Q.; Pan, W.; Barreteau, C.; Berardan, D.; Dragoe, N.; Zhao, L.-D. High Thermoelectric Performance of Oxyselenides: Intrinsically Low Thermal Conductivity of CaDoped BiCuSeO. *NPG Asia Mater.* 2013, **5**, No. e47.
219. Pei, Y.-L.; Wu, H.; Wu, D.; Zheng, F.; He, J. High Thermoelectric Performance Realized in a BiCuSeO System by Improving Carrier Mobility through 3D Modulation Doping. *J. Am. Chem. Soc.* 2014, **136**, 13902-13908.
220. Ren, G. K.; Butt, S.; Liu, Y. C.; Lan, J. L.; Lin, Y. H.; Nan, C. W.; Fu, F.; Tang, X. F. Enhanced Thermoelectric Performance of Zn-Doped Oxyselenides: BiCu1‑*x*Zn*x*SeO. *Phys. Status Solidi A* 2014, **211**, 2616-2620.
221. Ren, G.-K.; Butt, S.; Ventura, K. J.; Lin, Y.-H.; Nan, C.-W.; Lan, J.-L. Enhanced Thermoelectric Properties in Pb-Doped BiCuSeO Oxyselenides Prepared by Ultrafast Synthesis. *RSC Adv.* 2015, **5**, 69878-69885.
222. Sui, J.; Li, J.; He, J.; Pei, Y.-L.; Berardan, D.; Wu, H.; Dragoe, N.; Cai, W.; Zhao, L.-D. Texturation Boosts the Thermoelectric Performance of BiCuSeO Oxyselenides. *Energy Environ. Sci.* 2013, **6**, 2916-2920.
223. Yang, D.; Su, X.; Yan, Y.; Hu, T.; Xie, H.; He, J.; Uher, C.; Kanatzidis, M. G.; Tang, X. Manipulating the Combustion Wave during Self-Propagating Synthesis for High Thermoelectric Performance of Layered Oxychalcogenide Bi1‑*x*Pb*x*CuSeO. *Chem. Mater.* 2016, **28**, 4628-4640.
224. Zhang, M.; Yang, J.; Jiang, Q.; Fu, L.; Xiao, Y.; Luo, Y.; Zhang, D.; Cheng, Y.; Zhou, Z. Multi-Role of Sodium Doping in BiCuSeO on High Thermoelectric Performance. *J. Electron. Mater.* 2015, **44**, 2849-2855.
225. Liu, Y.; Zhao, L. D.; Zhu, Y.; Liu, Y.; Li, F.; Yu, M.; Liu, D. B.; Xu, W.; Lin, Y. H.; Nan, C. W. Synergistically Optimizing Electrical and Thermal Transport Properties of BiCuSeO via a Dual-Doping Approach. *Adv. Energy Mater.* 2016, **6**, 1502423.
226. Feng, B.; Li, G.; Pan, Z.; Hu, X.; Liu, P.; He, Z.; Li, Y.; Fan, X. Enhanced Thermoelectric Properties in BiCuSeO Ceramics by Pb/Ni Dual Doping and 3D Modulation Doping. *J. Solid State Chem.* 2019, **271**, 1-7.
227. Feng, B.; Li, G.; Pan, Z.; Hu, X.; Liu, P.; Li, Y.; He, Z.; Fan, X. Enhanced Thermoelectric Performances in BiCuSeO Oxyselenides via Er and 3D Modulation Doping. *Ceram. Int.* 2019, **45**, 4493-4498.
228. Tang, J.; Xu, R.; Zhang, J.; Li, D.; Zhou, W.; Li, X.; Wang, Z. H.; Xu, F.; Tang, G.; Chen, G. Light Element Doping and Introducing Spin Entropy: An Effective Strategy for Enhancement of Thermoelectric Properties in BiCuSeO. *ACS Appl. Mater. Interfaces* 2019, **11**, 15543-15551.
229. Ren, G.-K.; Wang, S.-Y.; Zhu, Y.-C.; Ventura, K. J.; Tan, X.; Xu, W.; Lin, Y.-H.; Yang, J.; Nan, C.-W. Enhancing Thermoelectric Performance in Hierarchically Structured BiCuSeO by Increasing Bond Covalency and Weakening Carrier-Phonon Coupling. *Energy Environ. Sci.* 2017, **10**, 1590-1599.
230. Li, F.; Ruan, M.; Chen, Y.; Wang, W.; Luo, J.; Zheng, Z.; Fan, P. Enhanced Thermoelectric Properties of Polycrystalline BiCuSeO via Dual-Doping in Bi Sites. *Inorg. Chem. Front.* 2019, **6**, 799-807.
231. Ren, G.-K.; Wang, S.; Zhou, Z.; Li, X.; Yang, J.; Zhang, W.; Lin, Y.-H.; Yang, J.; Nan, C.-W. Complex Electronic Structure and Compositing Effect in High Performance Thermoelectric BiCuSeO. *Nat. Commun.* 2019, **10**, 2814.
232. Li, F.; Zheng, Z.; Chang, Y.; Ruan, M.; Ge, Z.; Chen, Y.; Fan, P. Synergetic Tuning of the Electrical and Thermal Transport Properties via Pb/Ag Dual Doping in BiCuSeO. *ACS Appl. Mater. Interfaces* 2019, **11**, 45737-45745.
233. Deng, S.; Saiga, Y.; Kajisa, K.; Takabatake, T. High Thermoelectric Performance of Cu Substituted Type-VIII Clathrate Ba8Ga16-*x*Cu*x*Sn30 Single Crystals. *J. Appl. Phys.* 2011, **109**, 103704.
234. Saiga, Y.; Du, B.; Deng, S.; Kajisa, K.; Takabatake, T. Thermoelectric Properties of Type-VIII Clathrate Ba8Ga16Sn30 Doped with Cu. *J. Alloys Compd.* 2012, **537**, 303-307.
235. Chen, Y.-X.; Du, B.-L.; Saiga, Y.; Kajisa, K.; Takabatake, T. Crystal Growth and Thermoelectric Properties of Type-VIII Clathrate Ba8Ga15.9Sn30.1‑*x*Ge*x* with p-Type Charge Carriers. *J. Phys. D: Appl. Phys.* 2013, **46**, 205302.
236. Falmbigl, M.; Grytsiv, A.; Rogl, P.; Heinrich, P.; Royanian, E.; Bauer, E. Tuning of Band Gap and Thermoelectric Properties of Type-I Clathrate Ba8Ni*x*Zn*y*Ge46‑*x*‑*y*‑*z*Sn*z*. *J. Alloys Compd.* 2013, **567**, 65-72.
237. Koda, S.; Kishimoto, K.; Akai, K.; Asada, H.; Koyanagi, T. Thermoelectric and Transport Properties of Sintered n-Type K8Ba16Ga40Sn96 with Type-II Clathrate Structure. *J. Appl. Phys.* 2014, **116**, No. 023710.
238. Falmbigl, M.; Grytsiv, A.; Rogl, P.; Yan, X.; Royanian, E.; Bauer, E. Influence of Sn-Substitution on the Thermoelectric Properties of the Clathrate Type-I, Ba8Zn*x*Ge46‑*x*‑*y*Sn*y*. *Dalton T.* 2013, **42**, 2913-2920.
239. Du, B.; Saiga, Y.; Kajisa, K.; Takabatake, T. Thermoelectric Properties of p-Type Clathrate Ba8.0Ga15.9Zn*y*Sn30.1 Single Crystals with Various Carrier Concentrations. *Chem. Mater.* 2015, **27**, 1830-1836.
240. Kishimoto, K.; Koda, S.; Akai, K.; Koyanagi, T. Thermoelectric Properties of Sintered Type-II Clathrates (K,Ba)24(Ga,Sn)136 with Various Carrier Concentrations. *J. Appl. Phys.* 2015, **118**, 125103.
241. Chen, Y.; Du, B.; Kajisa, K.; Takabatake, T. Effects of In Substitution for Ga on the Thermoelectric Properties of Type-VIII Clathrate Ba8Ga16Sn30 Single Crystals. *J. Electron. Mater.* 2014, **43**, 1916-1921.
242. Sun, B.; Jia, X.; Huo, D.; Sun, H.; Zhang, Y.; Liu, B.; Liu, H.; Kong, L.; Liu, B.; Ma, H. Effect of High-Temperature and HighPressure Processing on the Structure and Thermoelectric Properties of Clathrate Ba8Ga16Ge30. *J. Phys. Chem. C* 2016, **120**, 10104-10110.
243. Wang, J.; Lebedev, O. I.; Lee, K.; Dolyniuk, J.-A.; Klavins, P.; Bux, S.; Kovnir, K. High-Efficiency Thermoelectric Ba8Cu14Ge6P26: Bridging the Gap between Tetrel-Based and Tetrel-Free Clathrates. Chem. Sci. 2017, 8, 8030-8038.
244. Wang, L.-H.; Chang, L.-S. Thermoelectric Properties of p-Type Ba8Ga16Ge30 Type-I Clathrate Compounds Prepared by the Vertical Bridgman Method. *J. Alloys Compd.* 2017, **722**, 644-650.
245. Deng, S.; Liu, H.; Li, D.; Wang, J.; Cheng, F.; Shen, L.; Deng, S. Thermoelectric Properties of Sr-Filled Ge-Based Type I Single-Crystal Clathrate Grown by Sn-Flux Method. *J. Electron. Mater.* 2017, **46**, 2662-2667.
246. Hou, Y.-H.; Chang, L.-S. Optimization on the Figure-of-Merit of p-Ttype Ba8Ga16Ge30 Type-I Clathrate Grown via the Bridgman Method by Fine Tuning Ga/Ge Ratio. *J. Alloys Compd.* 2018, **736**, 108-114.
247. Shen, L.; Li, D.; Deng, S.; Tang, Y.; Chen, Z.; Liu, Z.; Yang, P.; Deng, S. Preparation and Thermoelectric Properties of Zn-Doped SnBased Type-VIII Single-Crystalline Clathrate via a Grey Sn-Flux Method. *Cryst. Res. Technol.* 2018, **53**, 1700150.
248. Saiga, Y.; Suekuni, K.; Deng, S. K.; Yamamoto, T.; Kono, Y.; Ohya, N.; Takabatake, T. Optimization of Thermoelectric Properties of Type-VIII Clathrate Ba8Ga16Sn30 by Carrier Tuning. *J. Alloys Compd.* 2010, 507, 1-5.
249. Deng, S.; Saiga, Y.; Suekuni, K.; Takabatake, T. Enhancement of Thermoelectric Efficiency in Type-VIII Clathrate Ba8Ga16Sn30 by Al Substitution for Ga. *J. Appl. Phys.* 2010, **108**, No. 073705.
250. Anno, H.; Yamada, H.; Nakabayashi, T.; Hokazono, M.; Shirataki, R. Influence of Preparation Conditions on Thermoelectric Properties of Ba8Ga16Si30 Clathrate by Combining Arc Melting and Spark Plasma Sintering Methods. *J. Phys.: Conf. Ser.* 2012, **379**, No. 012007.
251. Kishimoto, K.; Yamamoto, H.; Akai, K.; Koyanagi, T. Effect of Ge Substitution on Carrier Mobilities and Thermoelectric Properties of Sintered p-Type Ba8Ga16+*x*Sn30‑*x*‑*y*Ge*y* with the Type-VIII Clathrate Structure. *J. Phys. D: Appl. Phys.* 2012, **45**, 445306.
252. Deng, S. K.; Saiga, Y.; Suekuni, K.; Takabatake, T. Effect of Al Substitution on the Thermoelectric Properties of the Type VIII Clathrate Ba8Ga16Sn30. *J. Electron. Mater.* 2011, **40**, 1124-1128.