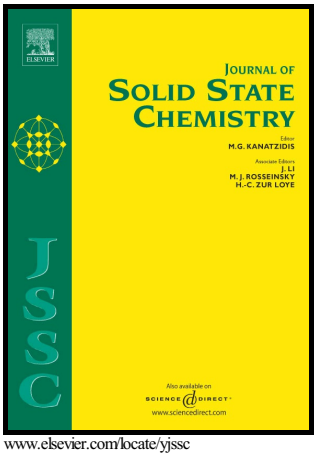

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Thermoelectric properties of Cu/Ag doped type-III $Ba_{24}Ge_{100}$ clathrates

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Abstract: Type-III $Ba_{24}Ge_{100}$ clathrates possess low thermal conductivity and high electrical conductivity at room temperature and, as such, have a great potential as thermoelectric materials for power generation. However, the Seebeck coefficient is very low due to the intrinsically high carrier concentration. In this paper, a series of $Ba_{24}Cu_xGe_{100-x}$ and $Ba_{24}Ag_yGe_{100-y}$ specimens were prepared by vacuum melting combined with the subsequent spark plasma sintering (SPS) process. Doping Cu or Ag on the Ge site not only suppresses the concentration of electrons but it also decreases the thermal conductivity. In addition, the carrier mobility and the Seebeck coefficient increase due to the decrease in the carrier concentration. Thus, the power factor is greatly improved, leading to an improvement in the dimensionless figure of merit *ZT*. Cu-doped $Ba_{24}Cu_6Ge_{94}$ reaches the maximum *ZT* value of about 0.17 at 873 K, while Ag-doped $Ba_{24}Ag_6Ge_{94}$ attains the dimensionless figure of merit *ZT* of 0.31 at 873 K, more than 2 times higher value compared to un-doped $Ba_{24}Ge_{100}$.

Graphical Abstract