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Enhanced thermoelectric performance in BiCuSeO Oxyselenides via Ba/Te dual-site substitution and 3D modulation doping

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Abstract:

Here, Bi_{1-x}Ba_xCuSe_{1-x}Te_xO ($x=0, 0.02, 0.04, 0.06, 0.08, 0.10$) ceramics have been prepared by mechanical alloying (MA) and resistance pressing sintering (RPS) process. The effects of Ba/Te doping on the thermoelectric properties have been investigated systematically. For Ba doping, it can tune the Fermi level and promote the band convergence, decreasing the band gap and significantly enhancing the carrier concentration; for the Te doping based on Ba doping, it can profoundly reduce the difference of electronegativity in (Cu₂Se²⁻)²⁻ layer, increase bond covalency, and then increase the electrical conductivity. The results indicate that the substitution of Ba/Te

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