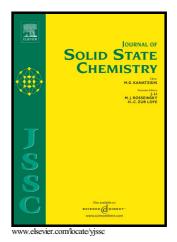
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PII:S0022-4596(18)30319-0DOI:https://doi.org/10.1016/j.jssc.2018.07.034Reference:YJSSC20315

To appear in: Journal of Solid State Chemistry

Received date: 20 May 2018 Revised date: 16 July 2018 Accepted date: 28 July 2018

Cite this article as: Bo Feng, Guangqiang Li, Zhao Pan, Xiaoming Hu, Peihai Liu, Zhu He, Yawei Li and Xi'an Fan, Enhanced thermoelectric performance in BiCuSeO Oxyselenides via Ba/Te dual-site substitution and 3D modulation d o p i n g , *Journal of Solid State Chemistry*, https://doi.org/10.1016/j.jssc.2018.07.034

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ACCEPTED MANUSCRIPT

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 $(Cu_2Se^2)^{2-}$ layer, increase bond covalency, and then increase the electrical conductivity. The results indicate that the substitution of Ba/Te Download English Version:

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