Low Lattice Thermal Conductivities and good thermoelectric performance of Hexagonal Antiperovskites X(Ba & Sr)$_3$BiN with Quartic Anharmonicity

Shuming Zeng,[1, *] Xiang Yan,[1] Qian Shen,[1] Yusong Tu,[1] Hao Huang,[2, †] and Geng Li[3, 4, ‡]

[1]*College of Physics Science and Technology,*

Yangzhou University, Jiangsu 225009, China

[2]*Advanced Copper Industry College,*

Jiangxi University of Science and Technology, Yingtan 335000,China

[3]*School of Materials Science and Engineering,*

National Institute for Advanced Materials, Nankai University,

Tongyan Road 38, Tianjin 300350, China.

[4]*National Supercomputer Center in Tianjin, Tianjin 300457, China.*

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* zengsm@yzu.edu.cn
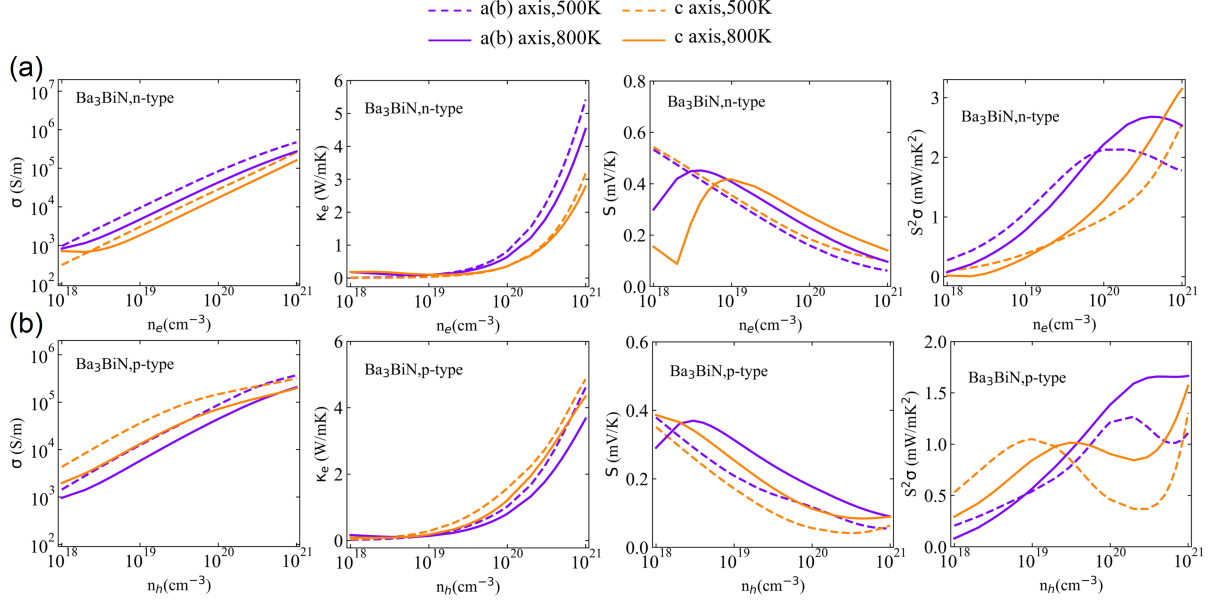
† huanghao201116@sina.cn

‡ ligeng@nscc-tj.cn

FIG. S1. The calculated electron conductivities σ, electronic thermal conductivity κ_e, Seebeck coefficient S, and power factor (PF), for n-type and p-type doping levels ranging from 1.0×10^{18} to $1.0 \times 10^{21} \mathrm{cm}^{-3}$, at 500 K and 800 K for Ba_3BiN.
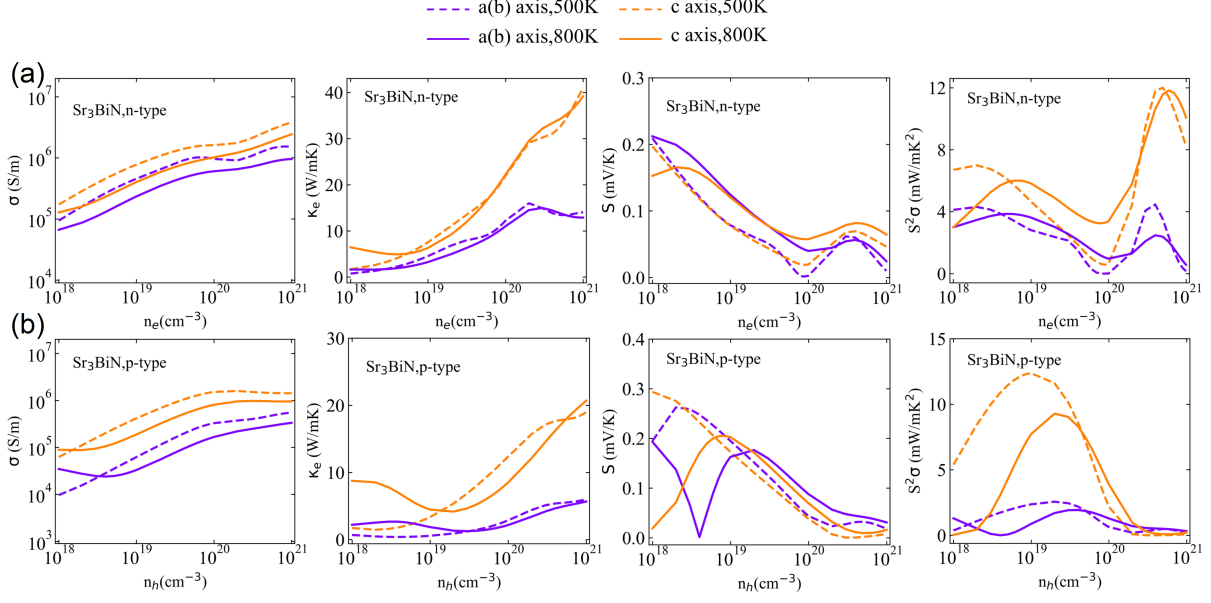
FIG. S2. The calculated electron conductivities σ, electronic thermal conductivity κ_e, Seebeck coefficient S, and power factor (PF), for n-type and p-type doping levels ranging from 1.0×10^{18} to 1.0×10^{21}cm^{-3}, at 500 K and 800 K for Sr$_3$BiN.
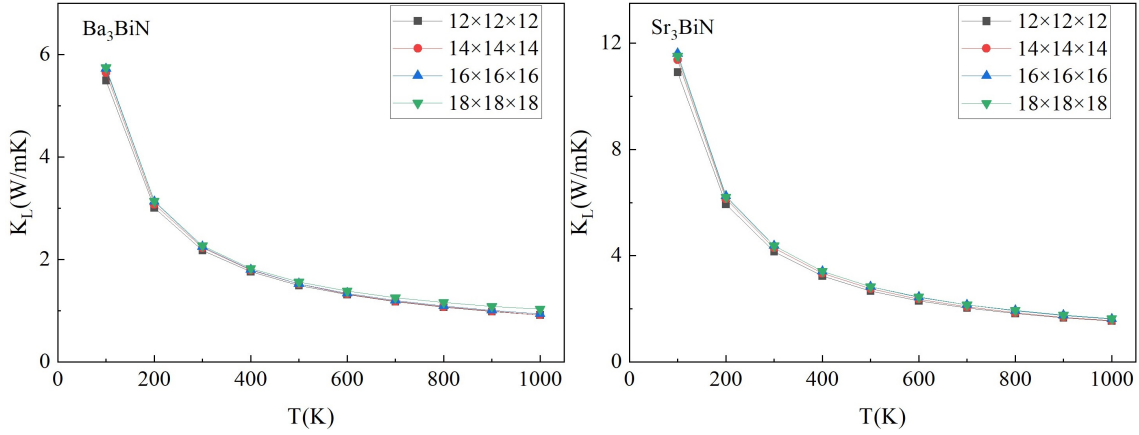

FIG. S3. The lattice thermal conductivities (κ_L) of Ba$_3$BiN and Sr$_3$BiN calculated with different q-points at different temperatures using SCP+BTE method. It can be concludede that the κ_L values converge when q-point density is greater than $16 \times 16 \times 16$ at temperatures range from 100 to 1000K.