Enhanced Thermoelectric Properties in a New Silicon Crystal Si_{24} with Intrinsic Nanoscale Porous Structure

Seoung-Hun Kang[1]
Kisung Chae[1], Seon-Myeong Choi[1], Duck Young Kim[2], and Young-Woo Son[1]

[1]*Korea Institute for Advanced study, Seoul 02455, South Korea*
[2]*Center for High Pressure Science & Technology Advanced Research, Shanghai 201203, People's Republic of China*

hand@kias.re.kr, duckyoung.kim@hpstar.ac.cn.

Thermoelectric device is a promising next-generation energy solution owing to its capability to transform waste heat into useful electric energy, which can be realized in materials with high electric conductivities and low thermal conductivities. A recently synthesized silicon allotrope of Si_{24} features highly anisotropic crystal structure with nanometer-sized regular pores. Here, based on first-principles study without any empirical parameter we show that the slightly doped Si_{24} can provide an order-of-magnitude enhanced thermoelectric figure of merit at room temperature, compared with the cubic diamond phase of silicon. We ascribe the enhancement to the intrinsic nanostructure formed by the nanopore array, which effectively hinders heat conduction while electric conductivity is maintained. This can be a viable option to enhance the thermoelectric figure of merit without further forming an extrinsic nanostructure. In addition, we propose a practical strategy to further diminish the thermal conductivity without affecting electric conductivity by confining rattling guest atoms in the pores.

References

Figures

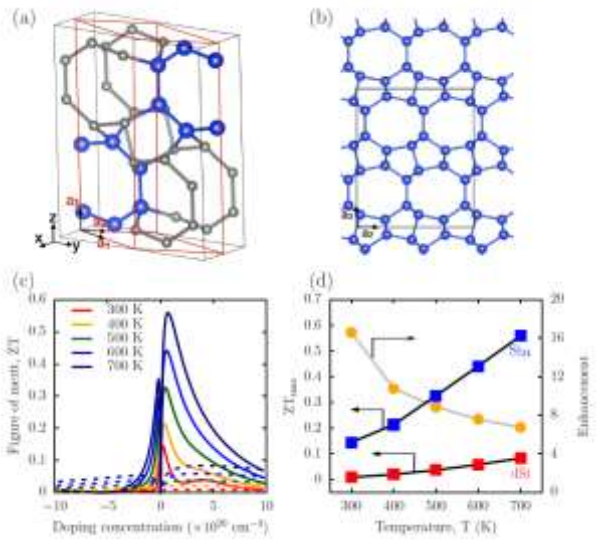

Figure 1: Ball-and-stick models of the Si_{24} crystal with (a) a perspective view and (b) orthogonal projection along the x-axis. (a) The primitive cell and the orthorhombic Bravais unitcell are shown as the red and black parallelepipeds, respectively. Twelve atoms in the primitive cell are shown in large blue balls, while the rest of the atoms are shown as small gray balls. (b) Continuous nanopores are shown where a one-dimensional array of Na ions (not shown) were confined for synthesis. (c) Thermoelectric figure of merit (ZT) of Si_{24} along x-axis are shown in continuous lines as a function of temperature, and the ZT values for dSi are also shown as dashed lines for comparison. Positive and negative doping concentrations (n) refer to that of excess electron and hole, respectively. (d) The maximum values of ZT (ZT_{max}) for a varying temperature are shown as squares, of which the optimum doping concentrations (in 10^{20} cm^{-3}) for Si_{24} are 0.21, 0.35, 0.44, 0.59 and 0.69 for increasing temperature; the values are 0.97, 1.81, 3.12, 3.43 and 4.03 for dSi. The enhancement (ratio of the ZT_{max} for Si_{24} to dSi) is also plotted as orange circles.