Supplemental Material

Strain-engineering the lattice thermal conductivity of 2D kagome silica

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For 2D linear elastic solid materials, the mechanical properties of x-y plane such as Young's modulus E can be expressed as following equations[1-3]:

$$E_x = \frac{C_{11}C_{22}-C_{12}C_{21}}{C_{22}},\ E_y = \frac{C_{11}C_{22}-C_{12}C_{21}}{C_{11}} \qquad \text{（S1）}$$

Table S1: Calculated values for elastic modulus tensor C_{ij} (in GPa) and Young's (in GPa) modulus E of 2D silica under different tensile strain.

Strain	C_{11}	C_{12}	C_{21}	C_{22}	E_x	E_y
0%	184.440	76.544	76.544	184.440	152.673	152.673
3%	172.232	64.484	64.484	172.232	148.089	148.089
8%	148.749	44.901	44.901	148.749	135.196	135.196

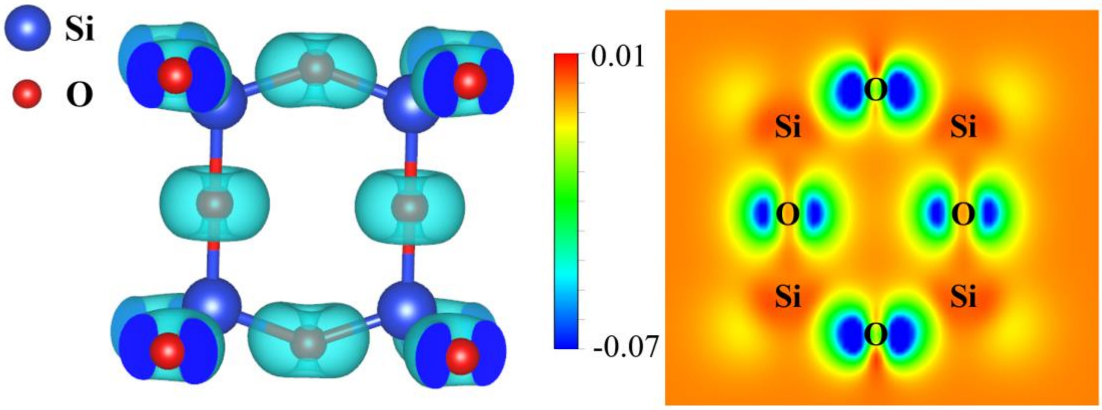

Fig S1. The charge density difference between the unstrained and 8% strained states, along with the 2D projection of the differential electron density function on the (110) plane.

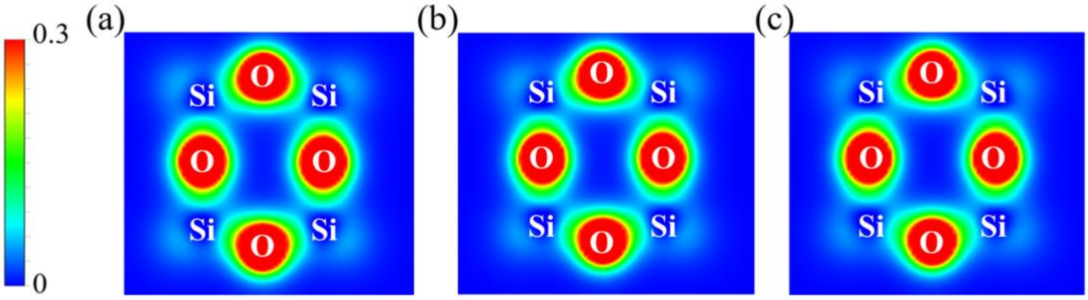

Fig S2. The effect of tensile strain on the electron density of nanocages. (a)-(c) show the 2D projections of the electron distribution density on the (110) plane for the structures without strain, under 3% strain, and under 8% strain, respectively.

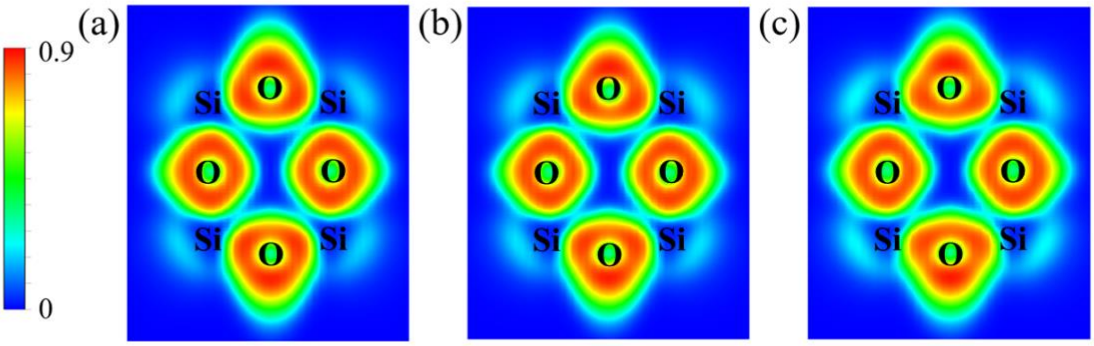

Fig S3. (a)-(c) 2D projections of the electron local function (ELF) on the (110) plane for the structures without strain, under 3% strain, and under 8% strain, respectively.

References:

[1] Q. Wei et al. *Appl. Phys. Lett.* **104,** 251915 (2014).
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[3] Z. Gao et al. *Nano Lett.* **17,** 772-777 (2017).