*Electronic Supplementary Information for*

# Tunable thermal transport in a $WS_2$ monolayer with isotopic doping and fractal structure

Dan Han [1], Wenyang Ding [1], Xinyu Wang [1,*], Lin Cheng [1,*]

[1] Institute of Thermal Science and Technology, Shandong University, Jinan 250061, China

## 1. Schematic of the NEMD approach and atomic configuration of $WS_2$ monolayer

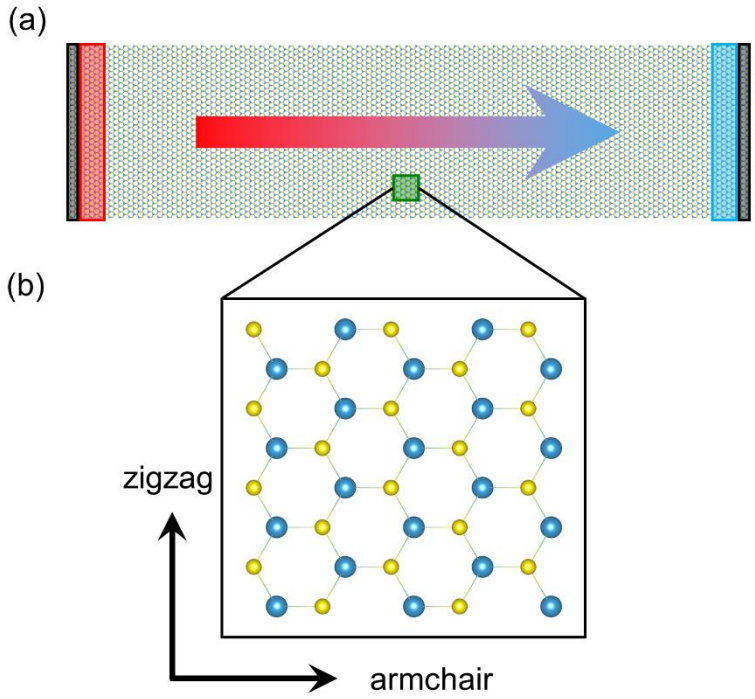


**Figure S1** (a) The schematic of the NEMD approach. The outmost black regions represent the fixed atoms at both ends with 3 Å. The red and blue regions show the heat source and sink with 10 Å. The arrow indicates the heat flux direction. (b) The zoom-in $WS_2$ monolayer structure of the olive region in (a). The blue solid spheres represent tungsten (W) atoms and the yellow spheres represent sulfur (S) atoms in $WS_2$ monolayer, respectively. In the simulation, the armchair and zigzag directions along the *x* and *y* directions, respectively.

Corresponding authors. Lin Cheng, Email: cheng@sdu.edu.cn; Xinyu Wang, Email: xyw@sdu.edu.cn.

## 2. Effect of system size

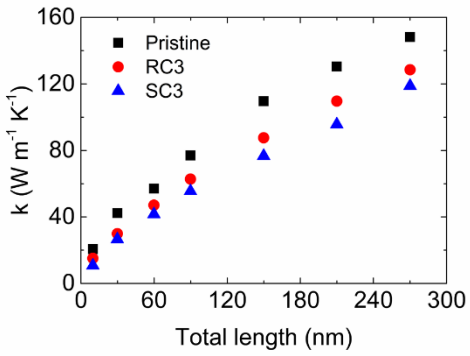


**Figure S2** Thermal conductivity variations of pristine, RC3 and SC3 $WS_2$ monolayers with different system lengths from 10.01 to 270.27 nm. It can be observed that the relationship of thermal conductivity is pristine>RC3>SC3 $WS_2$ monolayer at the same system length. Therefore, to save computational time, we choose 90.09×9.95 $nm^2$ as a representative total length in all MD simulation.

## 3. Isotopic doping atom concentrations with different fractal numbers

**Table S1** A summary of isotopic doping atom concentrations in RC and SC fractal structures.

| Fractal number | Isotopic doping atom concentration (%) | |
|---|---|---|
| | RC | SC |
| 0 | 0 | 0 |
| 1 | 10.8 | 10.8 |
| 2 | 20.5 | 20.4 |
| 3 | 28.9 | 29.1 |
| 4 | 36.9 | 36.7 |
| 5 | 43.0 | 43.7 |
| 6 | 47.0 | 47.5 |
| 7 | 52.4 | 52.8 |
| 8 | 55.6 | 56.3 |

## 4. Phonon bandgaps of pristine, RC2 and SC2 structures

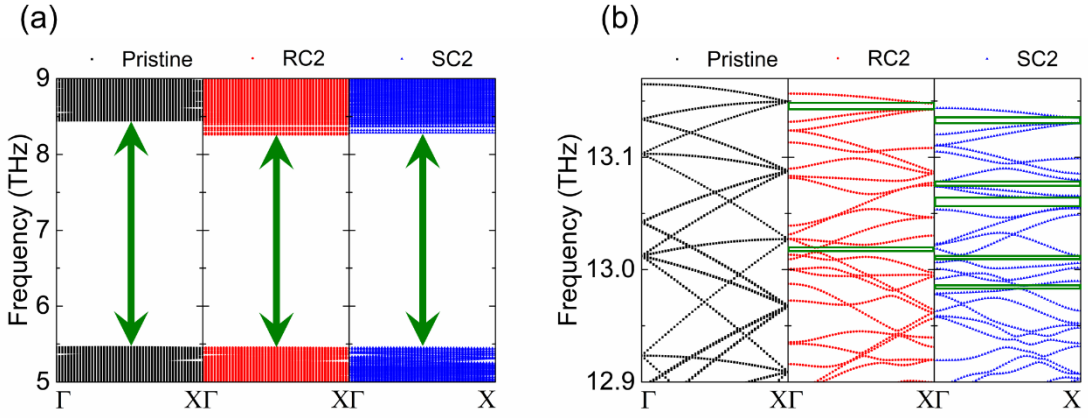


**Figure S3** Phonon bandgaps of pristine, RC2 and SC2 structures calculated from lattice dynamics using GULP. Phonon dispersions of (a) frequency region from 5 to 9 THz and (b) high frequency region from 12.9 to 13.17 THz. The olive arrows in (a) and olive boxes in (b) indicate the phonon bandgaps.

## 5. Group velocities in RC and SC structures with different fractal numbers

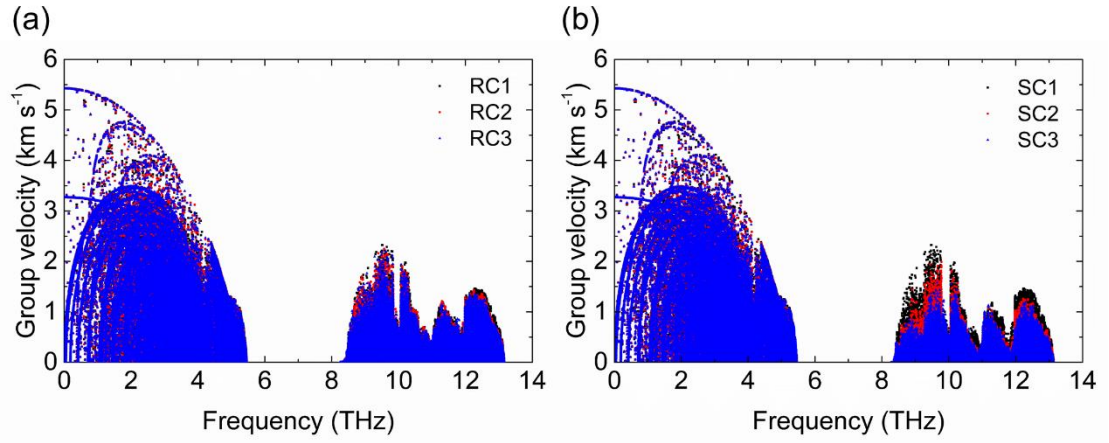


**Figure S4** Phonon group velocities of (a) RC1, RC2 and RC3 structures and (b) SC1, SC2 and SC3 structures calculated from phonon dispersions. At whole frequency region, the average group velocities of RC1, RC2 and RC3 structures are 423.31 m $s^{-1}$, 412.26 m $s^{-1}$ and 405.93 m $s^{-1}$, and the corresponding values of SC1, SC2 and SC3 structures are 423.31 m $s^{-1}$, 375.89 m $s^{-1}$ and 355.13 m $s^{-1}$, respectively.