纳米工程热传导和热电转换研究中的新思路

New Ideas on Thermal Conduction &Thermoelectics in Nano-Engineering

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http://energy.hust.edu.cn/nanoheat/


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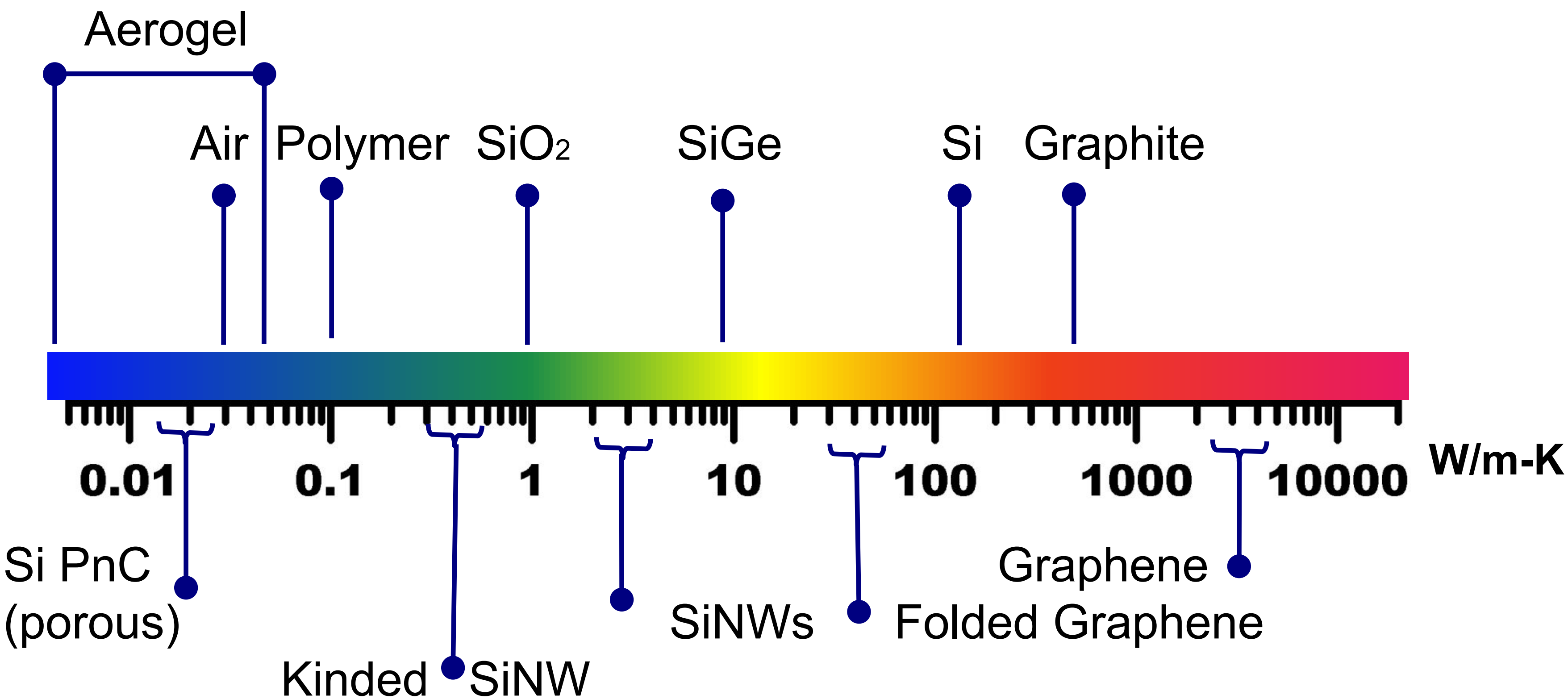
華中科技大學
HUAZHONG UNIVERSITY OF SCIENCE & TECHNOLOGY

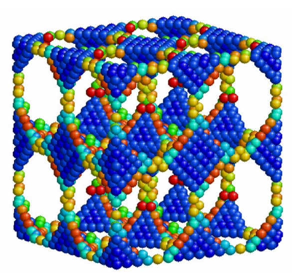
•提纲 Outline

- 1. 背景
  - 1.1 热导率
  - 1.2 应用
- 2. 纳米尺度传热
  - 2.1 纳米管聚乙烯链阵列
  - 2.2 石墨烯圆盘&二硫化钼
  - 2.3 分子晶体

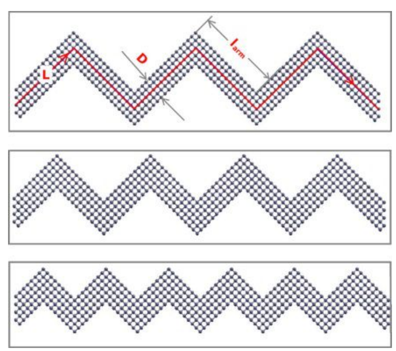
- 1. Background
  - 1.1 Thermal conductivity
  - 1.2 Applications
- 2. Nano Heat transfer
  - 2.1 1D CNT-PE array
  - 2.2 2D Graphene & $SLMoS_2$
  - 2.3 3D molecular crystals

1.1 热导率 Thermal conductivity

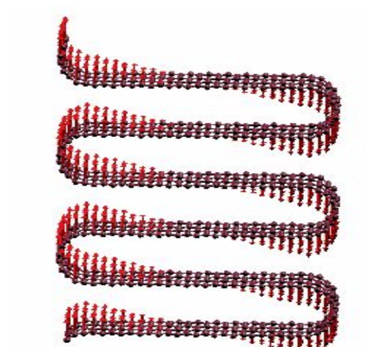




Nano Lett. 14, 1734 (2014)



Nano Lett. 13, 1670(2013)



Appl Phys Lett 100, 093107 (2012)

1.1 热导率 Thermal conductivity

Joseph Fourier (1768 –1830)

- Fourier's law:
  - The law of heat conduction:

$$\vec{J} = -\kappa \nabla T$$

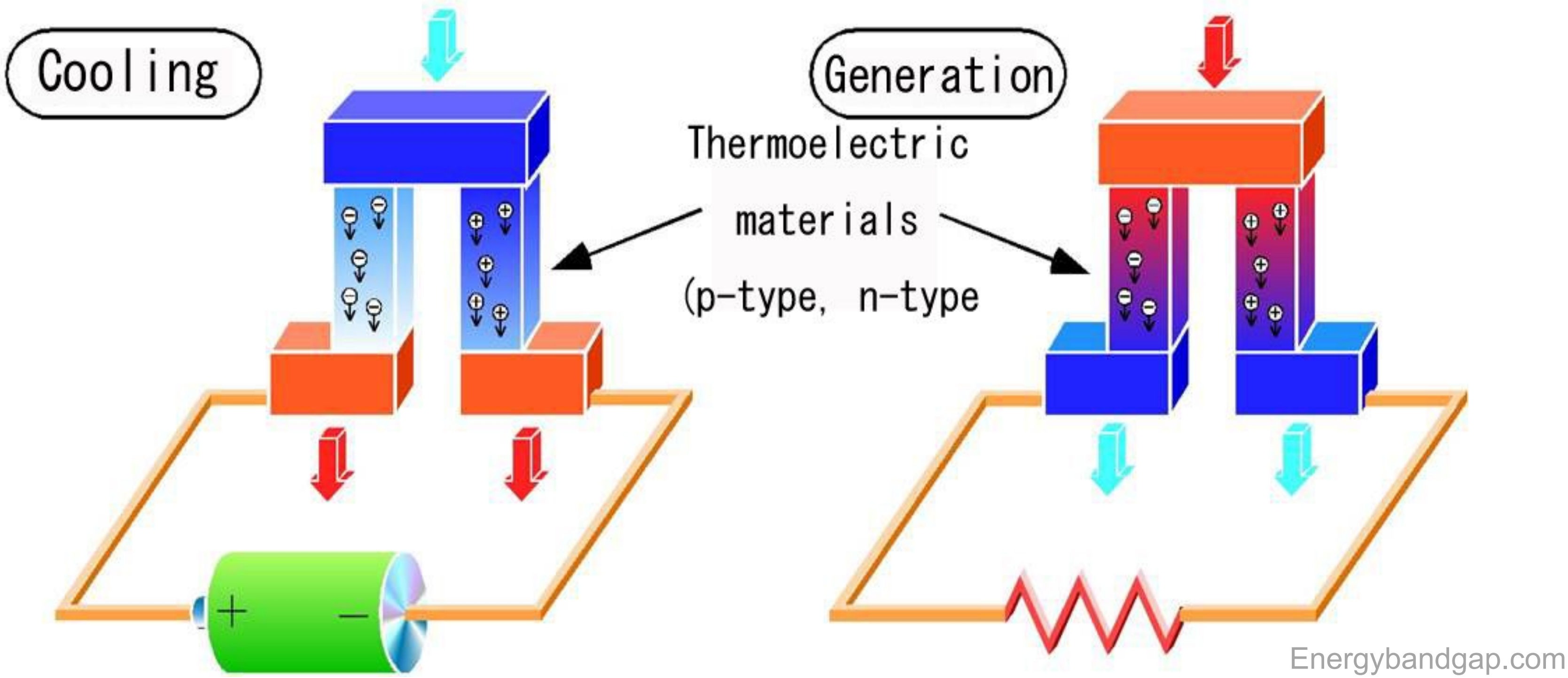
$\vec{J} \equiv \vec{q}$: heat flux density $[W/m^2]$

∇T: temperature gradient $[K/m]$

κ: thermal conductivity $[W/m-K]$

- κ is constant !...?
- Dependent on T, orientation
- Independent of SIZE

1.2 应用: 热电材料　Thermoelectric (TE)



$$zT = \frac{S^2\sigma}{\kappa}T$$

$S = -\Delta T / \Delta V$: Seebeck coecient

σ : electric conductivity

Thomas Seebeck
1770-1831

1.2 应用: 热电材料　Thermoelectric (TE)

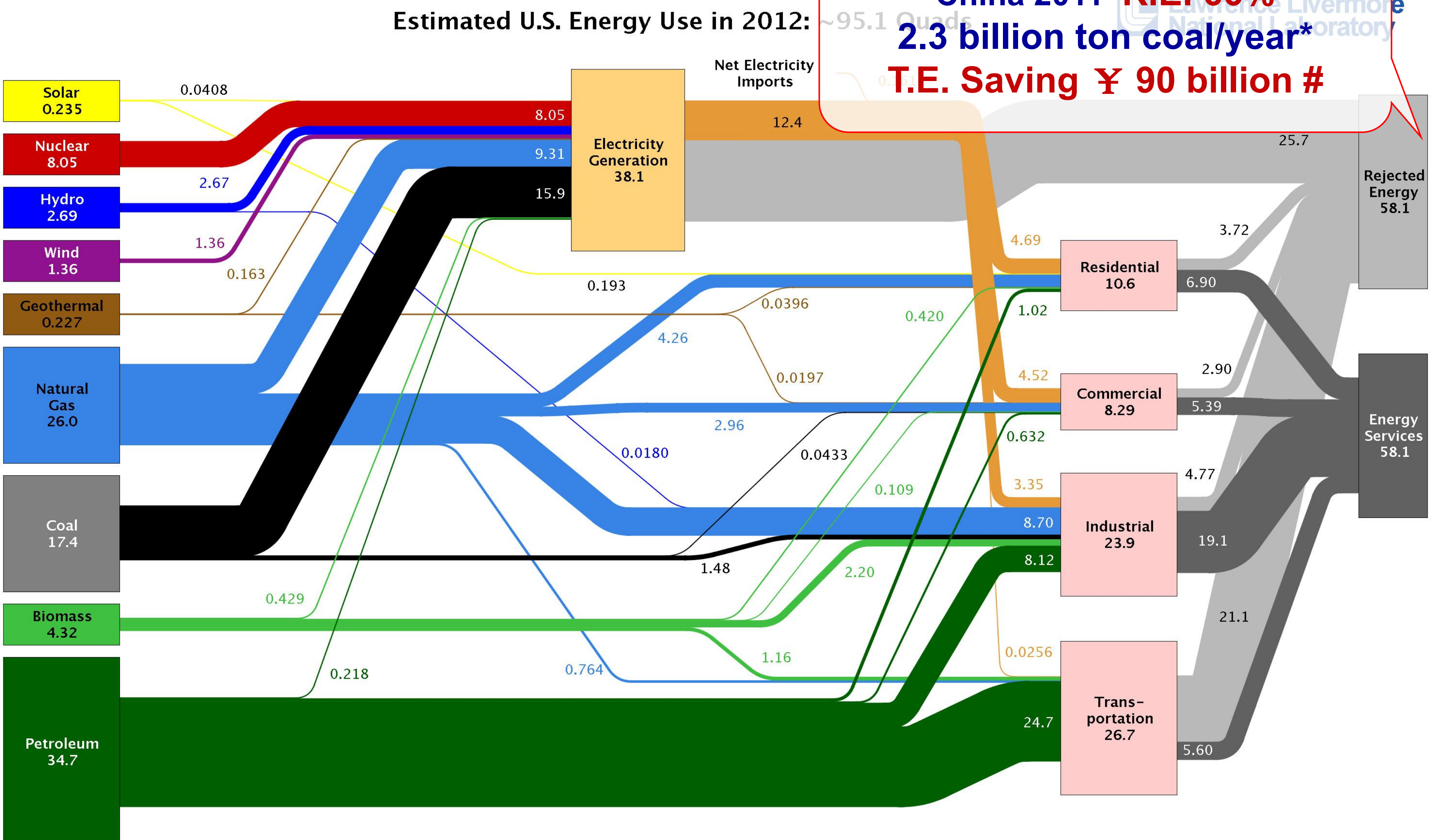
- 低噪音
- 大容量
- 便携小巧
- 冷暖两用
- 极速制冷
- 无制冷剂
- 省电？
- 0.5度/天 10L (1-8 ^{o}C)

vs

传统冰箱 0.5度/天 220L

1.2 应用: 热电材料 Thermoelectric (TE)

China 2011 R.E. 66%
2.3 billion ton coal/year*
T.E. Saving ￥ 90 billion #

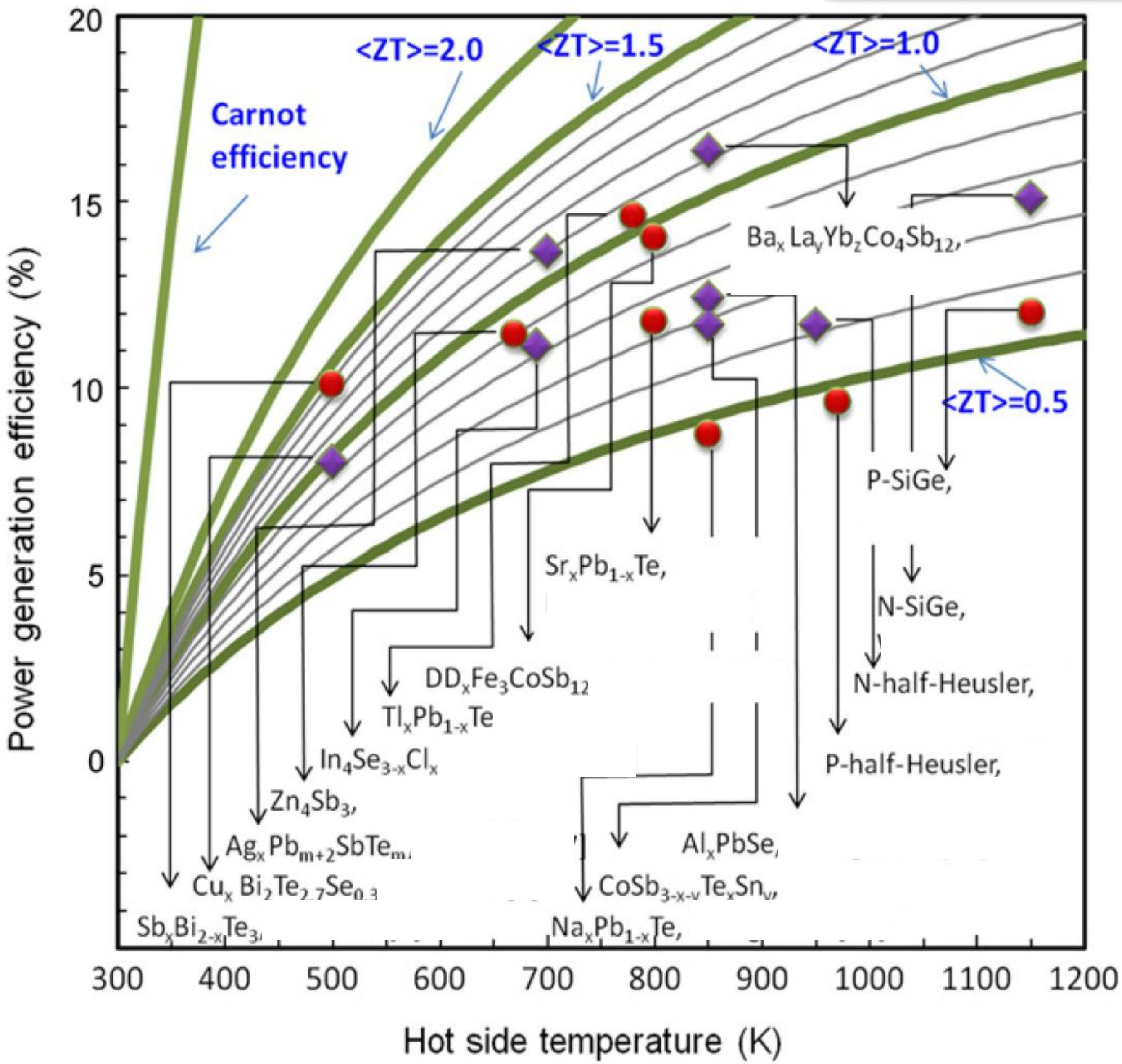


Source: LLNL 2013. Data is based on DOE/EIA-0035(2013-05), May, 2013. If this information or a r
and the Department of Energy, under whose auspices the work was performed. Distributed electri
consumption of renewable resources (i.e., hydro, wind, geothermal and solar) for electricity in BTU-equival
is calculated as the total retail electricity delivered divided by the primary energy input into electricity g
for the industrial sector, and 21% for the transportation sector. Totals may not

* 2012 Energy development report of China
\# T.E. effeciency 5%, 50% R.E. recovered, thermal power generation ￥0.2/kW-h

State of the art in TE

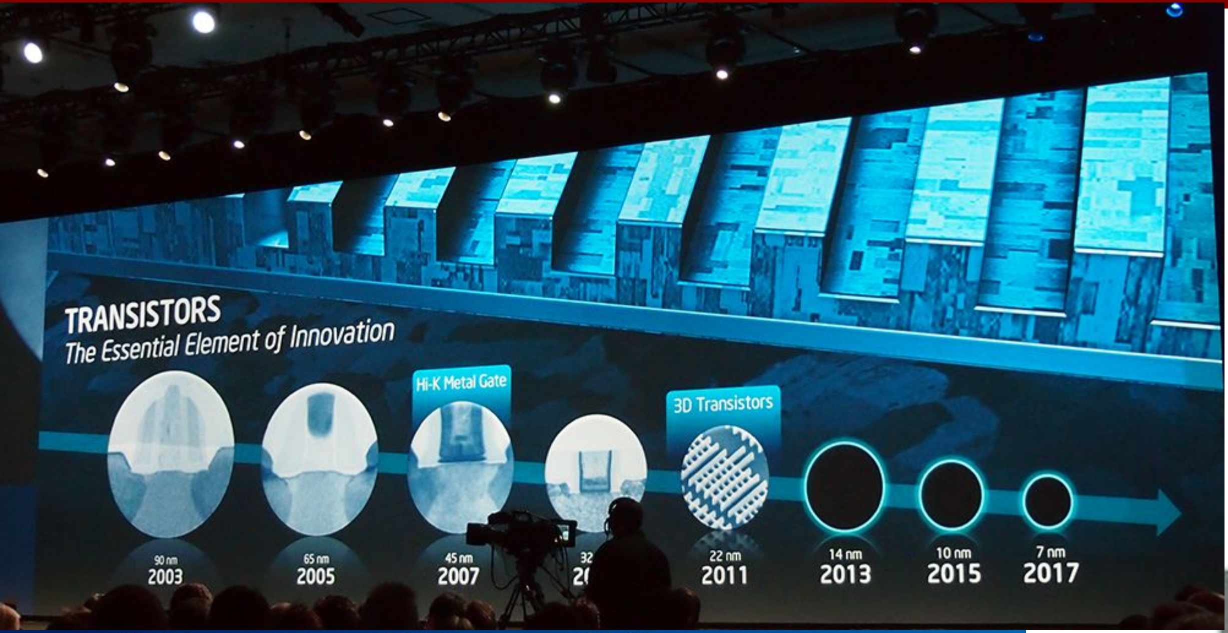
$$\eta_{max} = \frac{(T_H - T_C)(\sqrt{1 + ZT_M} + 1)}{T_H(\sqrt{1 + ZT_M} + T_C/T_H)}$$

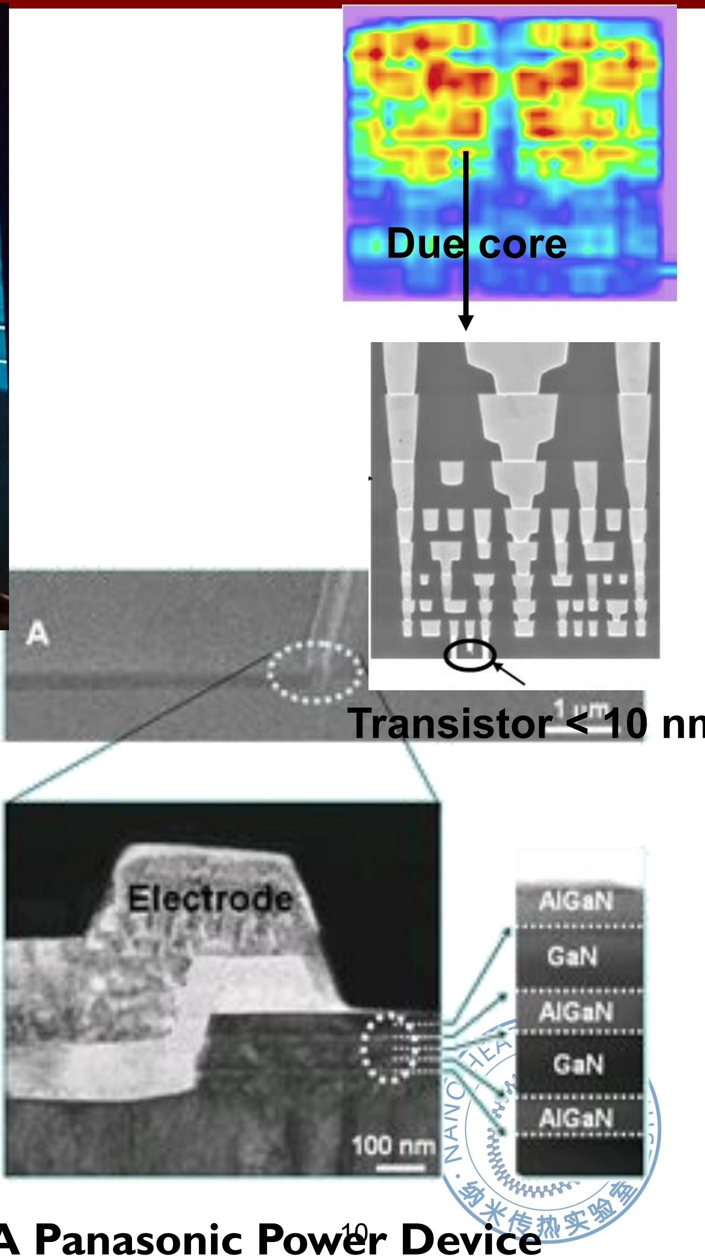


$$ZT = \frac{S^2\sigma}{\kappa}T$$

W. Liu, X. Yan, G. Chen, and Z. Ren, Nano Energy 1, 42 (2012).

•1.2 应用: 散热　　Heat removel





- Faster computers run **Hotter**
- Heat removel
  - Inside the chip (nanoscale)
  - Via thermal interface material
- Temperature drop across interfaces

A Panasonic Power Device

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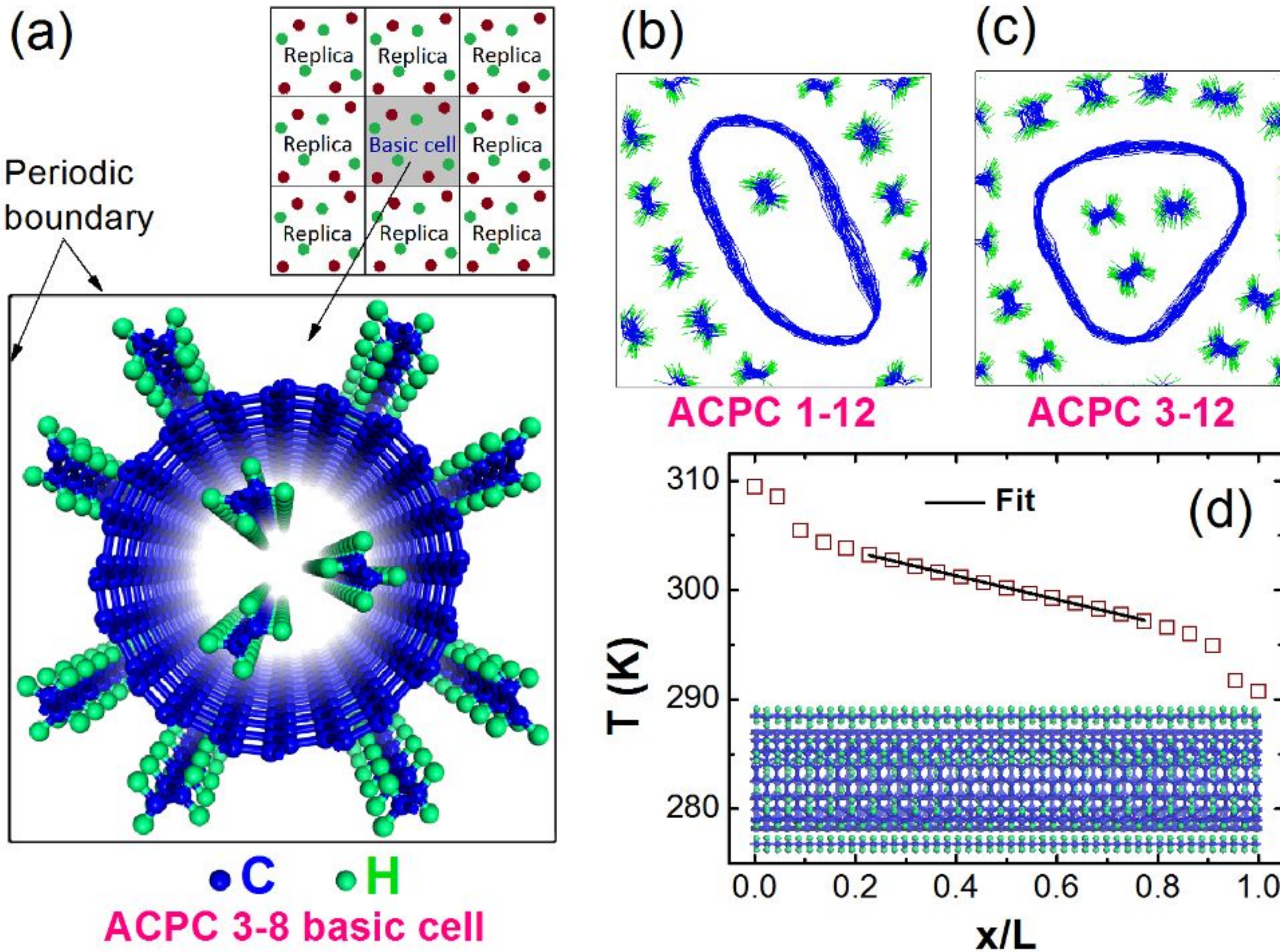
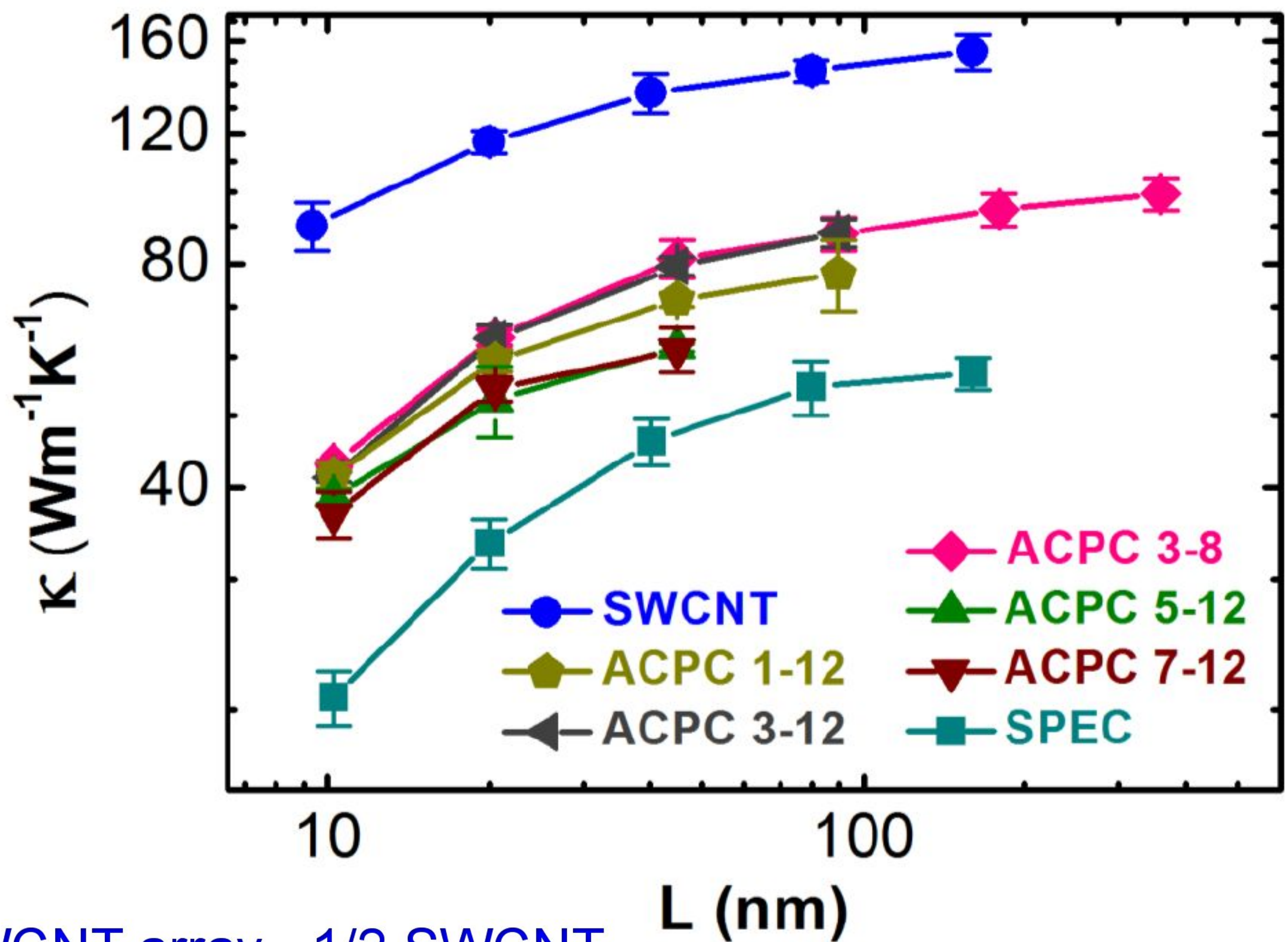
  - 2.3 3D molecular crystals

2.1 1D: High Thermal Conductivity of Aligned Carbon Nanotube-Polyethylene Array -- Scientific Reports 5, 16543 (2015)

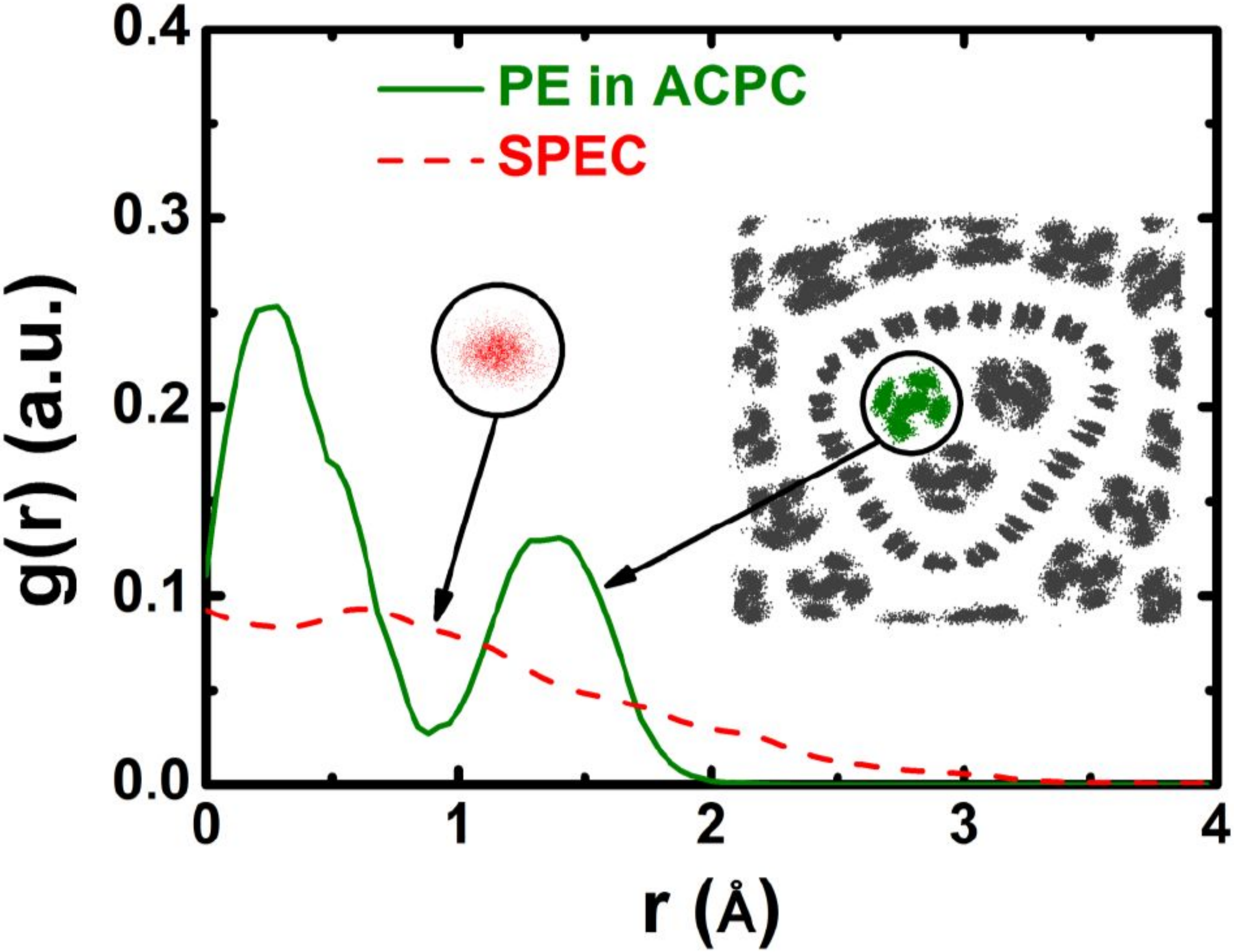


•Thermal conductivities vs length

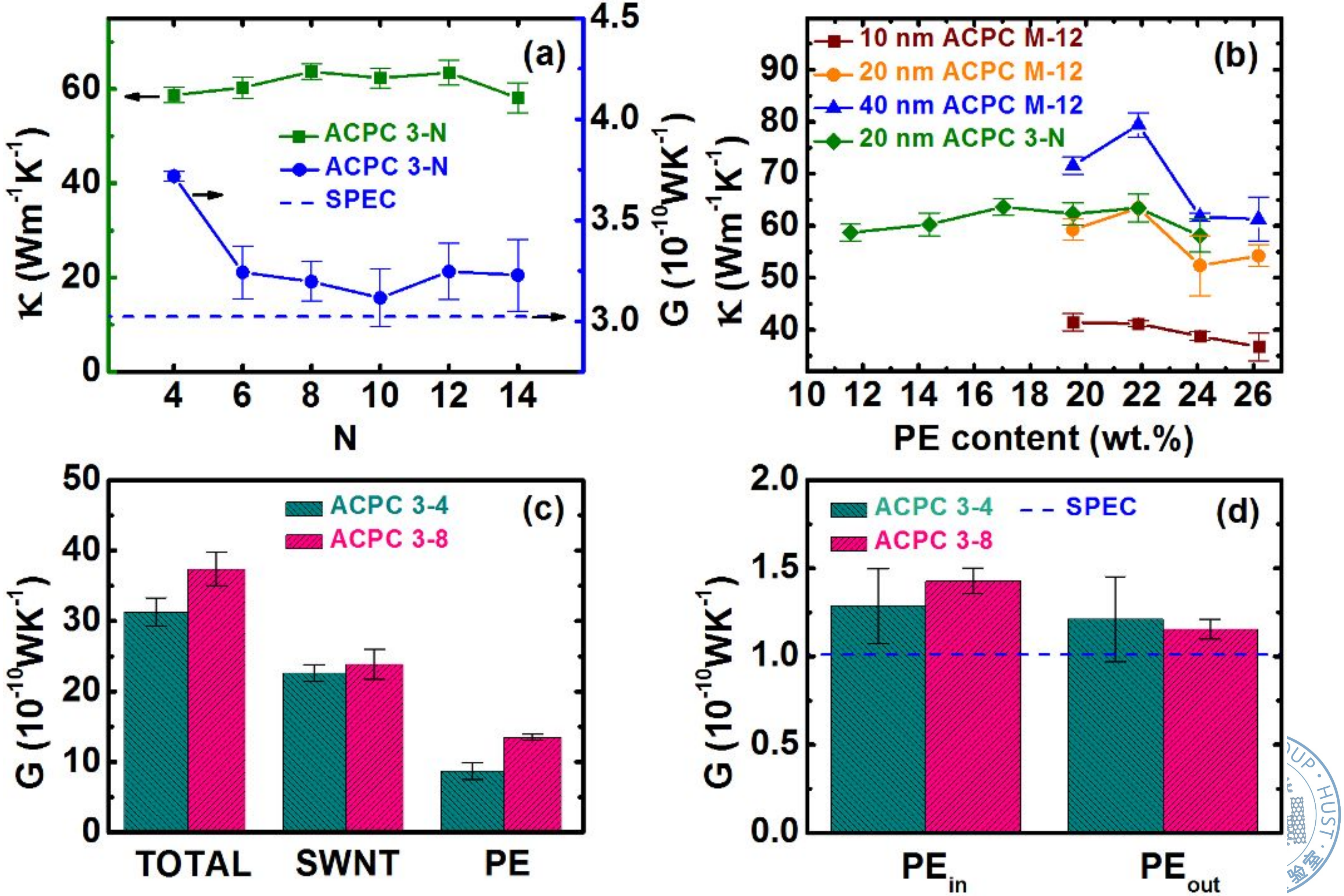


SWCNT array ~1/2 SWCNT

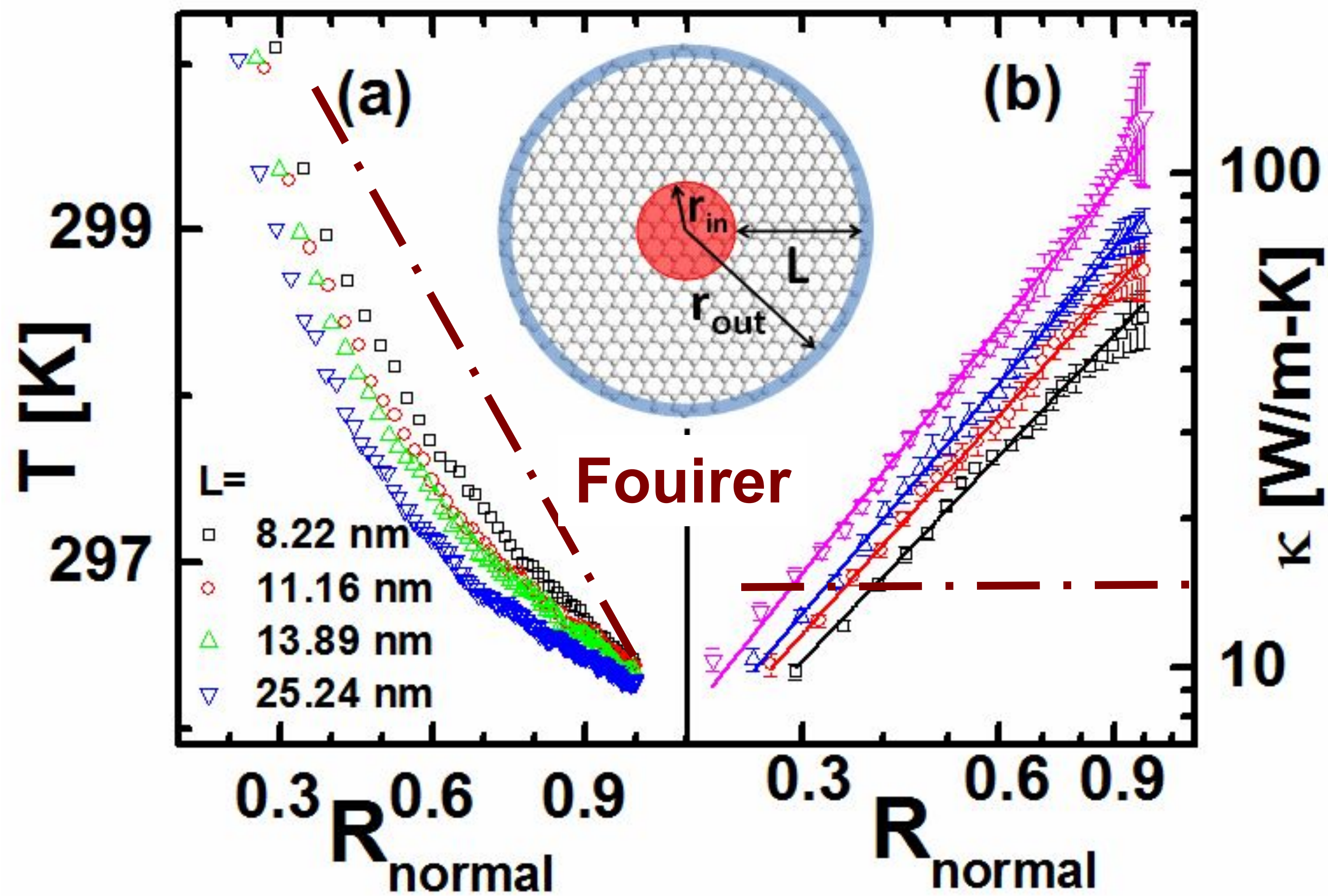
•The radial atomic density profiles, g(r)



Thermal conductivity and thermal conductance



2.2 2D: Nanoscale Graphene Disk: A Natural Graded Material -- Scientific Reports 5, 14878 (2015)



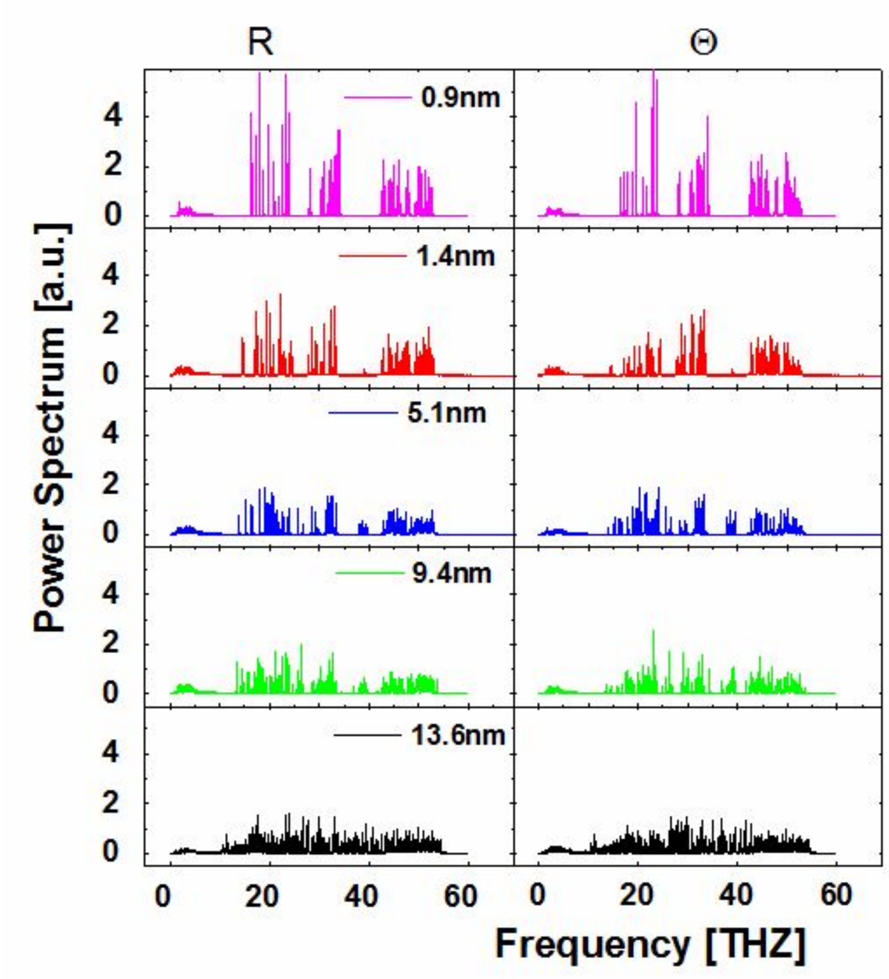
$$\kappa(r) = \kappa_0 \left[\frac{ln(C/r)}{ln(C/r_{out})} \right]^{\alpha} = \kappa_0 \left[\mathrm{R}_{normal}(\mathrm{r}) \right]^{\alpha}$$

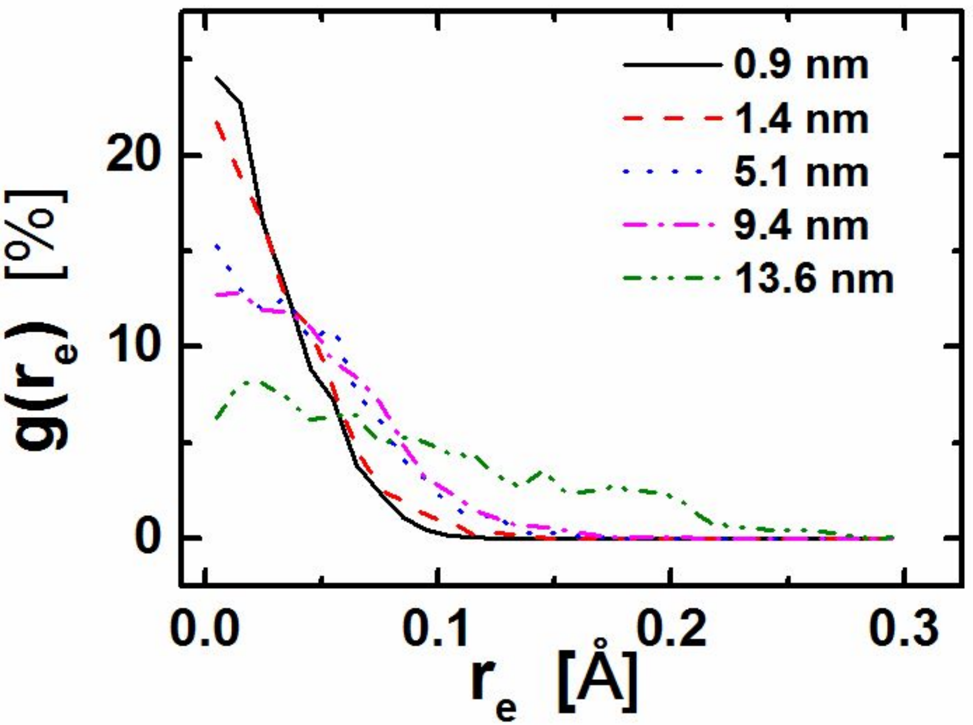
$$\mathrm{R}_{normal}(\mathrm{r}) = \frac{ln(C/r)}{ln(C/r_{out})}$$

where κ_0 and C are constants, and α is power-law exponent fitted from MD results.

$$T(r) = \begin{cases} T(r_{in}) + [T(r_{out}) - T(r_{in})] \dfrac{\mathrm{R}_{normal}(\mathrm{r})^{1-\alpha} - [\ln(r_{in}/C)/\ln(r_{out}/C)]^{1-\alpha}}{1 - [\ln(r_{in}/C)/\ln(r_{out}/C)]^{1-\alpha}}, \alpha \neq 1 \\ T(r_{in}) + [T(r_{out}) - T(r_{in})] \dfrac{\mathrm{R}_{normal}(\mathrm{r}) - [\ln(r_{in}/C)/\ln(r_{out}/C)]}{1 - [\ln(r_{in}/C)/\ln(r_{out}/C)]}, \alpha = 1 \end{cases}$$

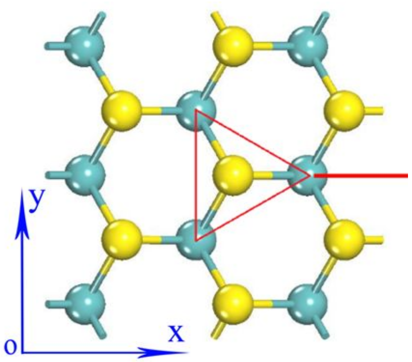
•Mechanism


R
Θ
0.9nm
1.4nm
5.1nm
9.4nm
13.6nm
Power Spectrum [a.u.]
Frequency [THZ]
0
2
4
20
40
60

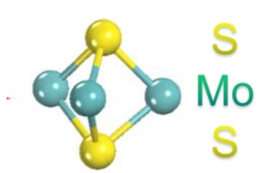

0.9 nm
1.4 nm
5.1 nm
9.4 nm
13.6 nm
g(r_e) [%]
r_e [Å]
0
10
20
0.0
0.1
0.2
0.3

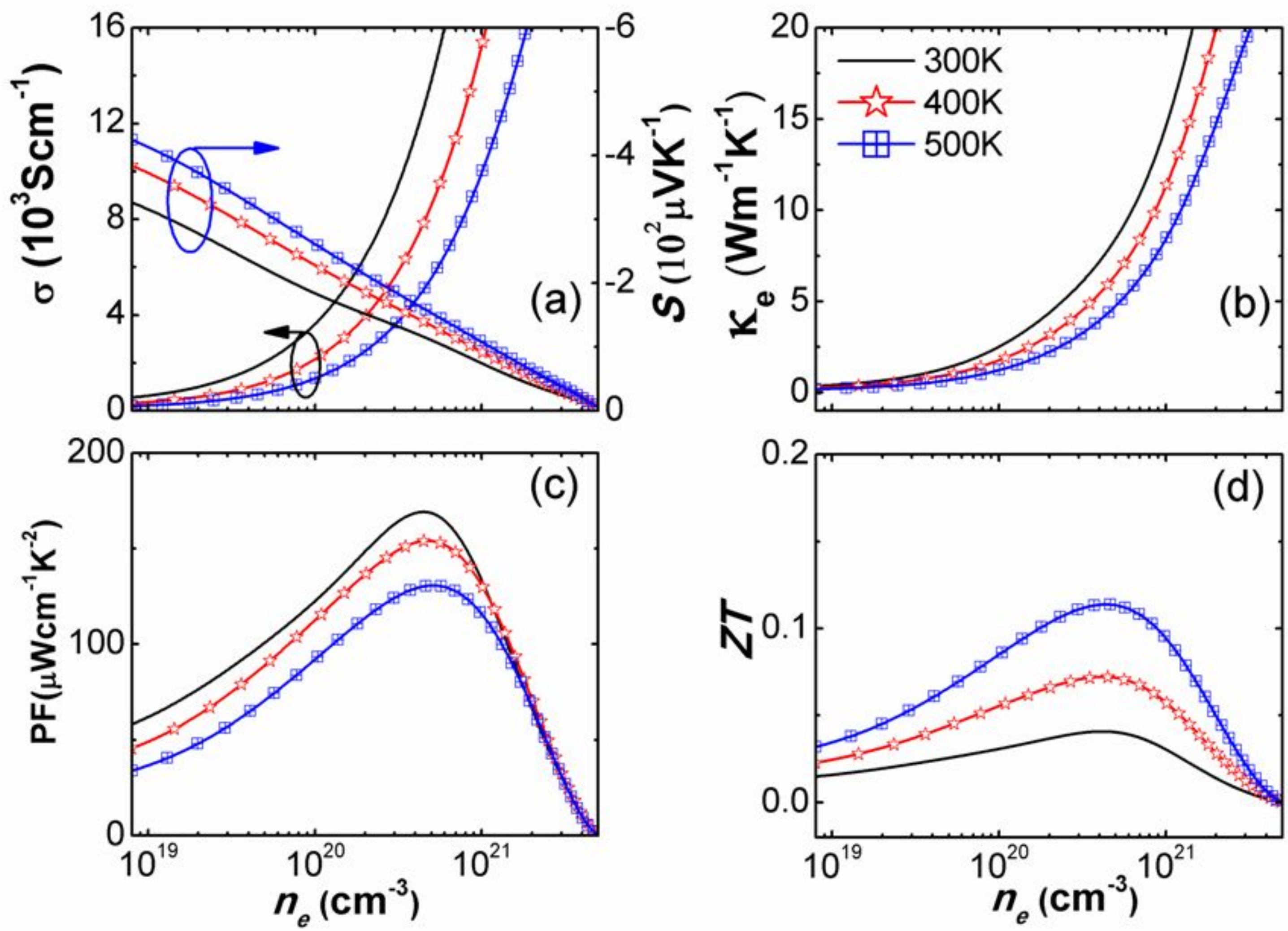
2.2 2D: A Revisit to Thermoelectric Performance of Single-layer MoS_2 arXiv:1504.03852

Top view



Side View

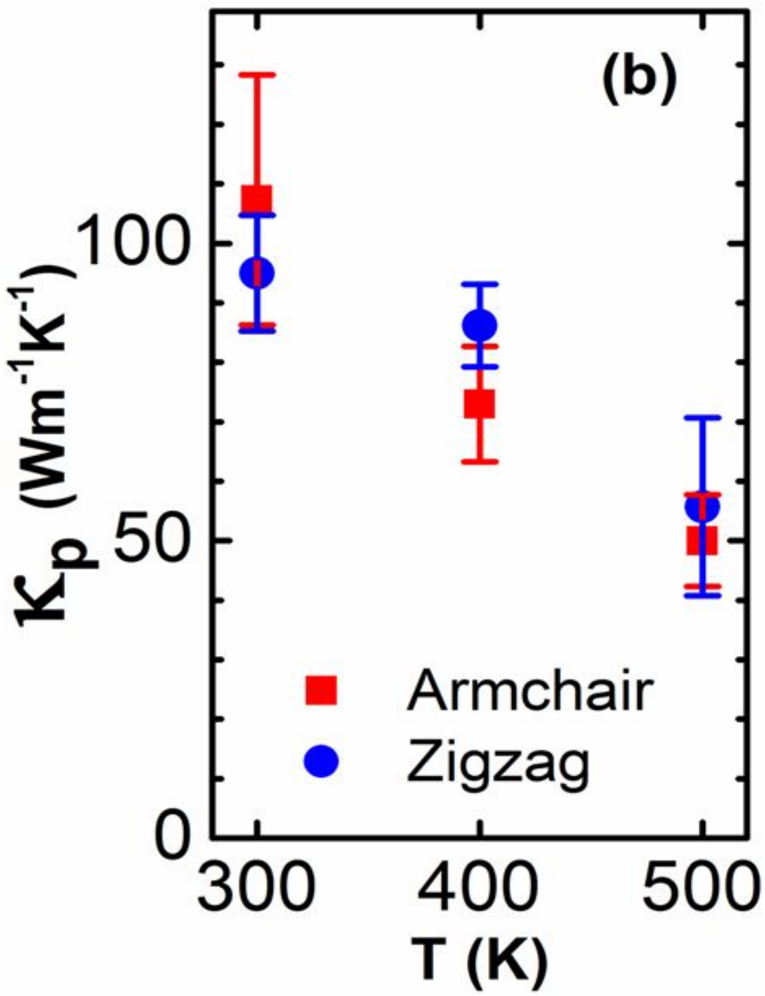


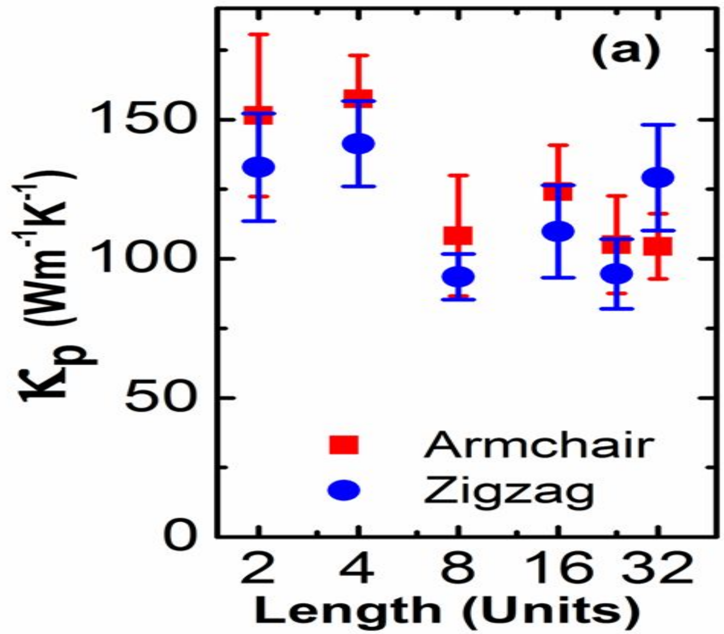


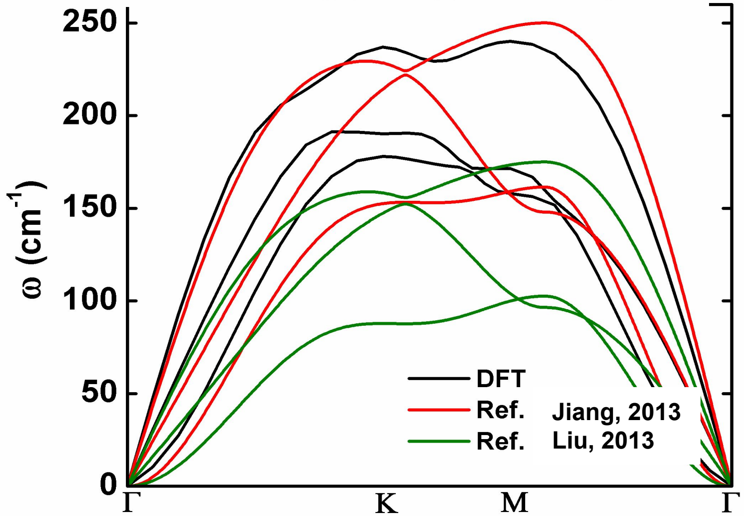
Comparison of thermoelectric properties

Struct.& Ref.	Method	T (K)	Carrier type	σ (Scm^{-1})	S (μVK^{-1})	κ_e ($Wm^{-1}K^{-1}$)	κ_{ph} ($Wm^{-1}K^{-1}$)	ZT
SL	DFT+BTE+MD	300	n p	14625 16957	-110 72.9	8.94 11.39	116.8	0.04 0.02
		500	n p	11714 8853	-161 150	9.69 8.40	52.9	0.26 0.16
SL[23]	DFT+Ballistic model	300	n p	54 108	-202 215	0.021 0.040	0.243 0.244	0.25 0.53
SLR[24,27]	DFT+BTE+MD	300	n p	7770 14300	-204 223	2.89 5.20	1.02	2.5 3.4
SL CVD[25]	Experiment	300	-	-	≤30000	-	-	-
SL FET[59]	Experiment	300	-	-	400-100000	-	-	-
Bulk[60]	Experiment	90-873	-	-	500-700	-	-	-
SL[27]	EMD	300	-	-	-	-	1.35	-
SL[30]	DFT+BTE	300	-	-	-	-	> 83	-
SL[28]	DFT+NEGF	300	-	-	-	-	23.2	-
SLR[29]	DFT+BTE	300	-	-	-	-	26.2	-
SLR[26]	NEMD	300	-	-	-	-	5	-
FL[31]	Experiment	300	-	-	-	-	52	-
SL[32]	Experiment	300	-	-	-	-	35.4	-
Bulk[33]	Experiment	300	-	-	-	-	85-110	-

•Thermal conductivity of $SLMoS_2$



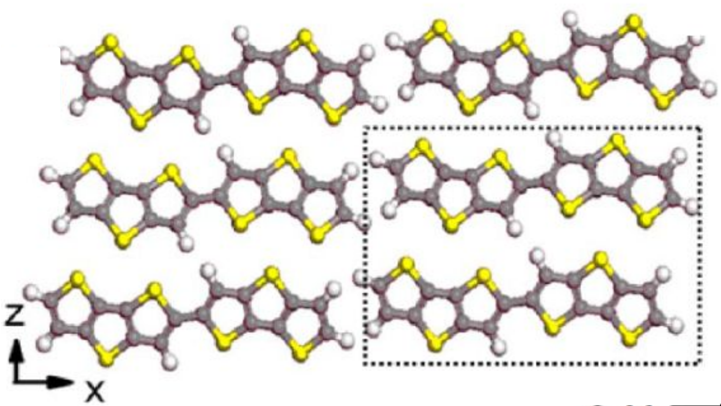


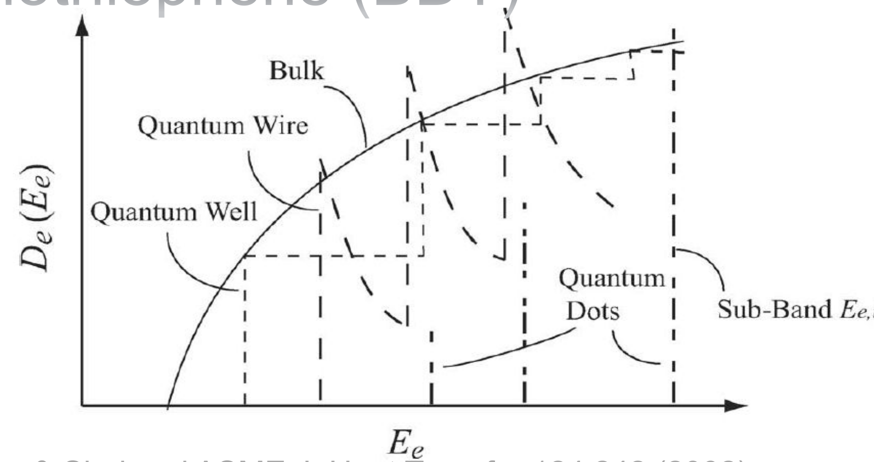


2.3 3D: Enhancing zT by Low-Dimensional Electrical Transport in Phonon-Glass Crystals Nano Letters 15, 5229 (2015)

Molecular Crystal : Bis-Dithienothiophene (BDT)

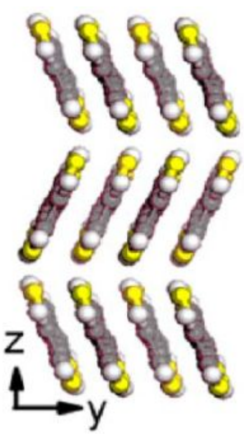
Top view $C_{16}H_6S_6$

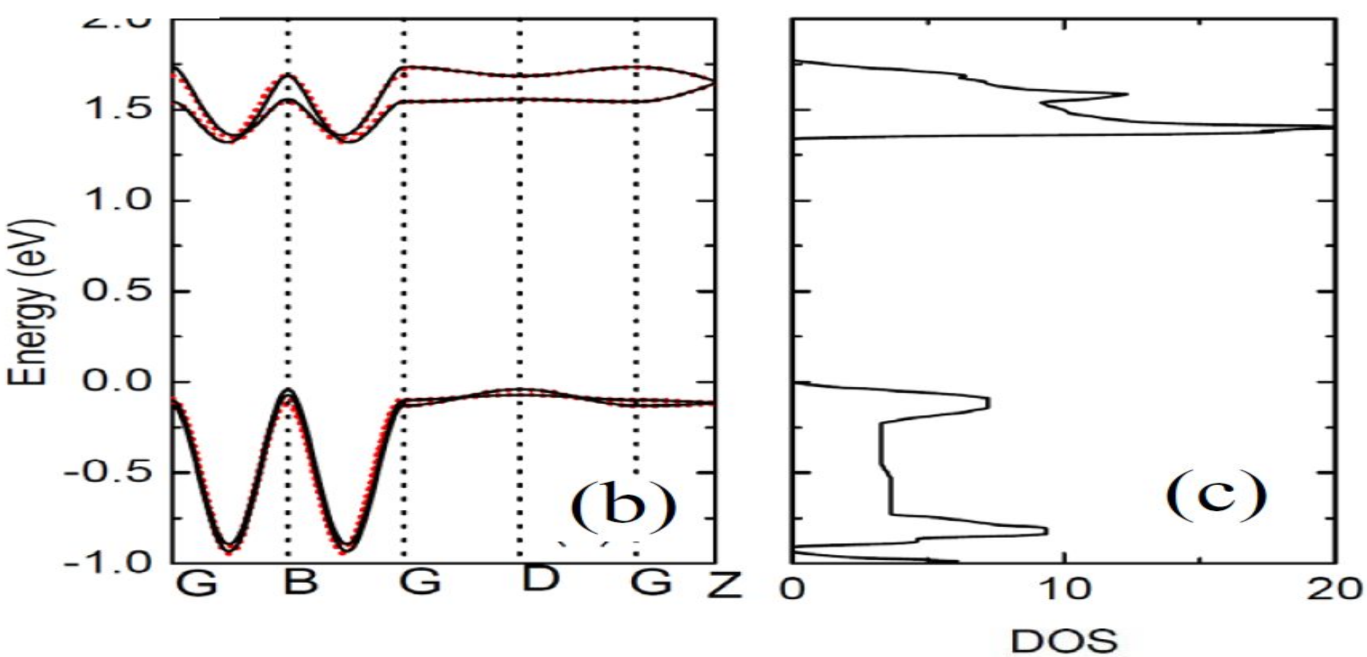




Chen & Shakouri ASME J. Heat Transfer 124 242 (2002)

Side View





• Thermoelectric Performance of BDT

	n $10^{20}cm^{-3}$	S μ V/K	κ_e W/m-K	κ_{ph} W/m-K	ZT
p-type	1.57	266	0.15	0.34	1.48
n-type	3.19	-199	0.06	0.34	0.38

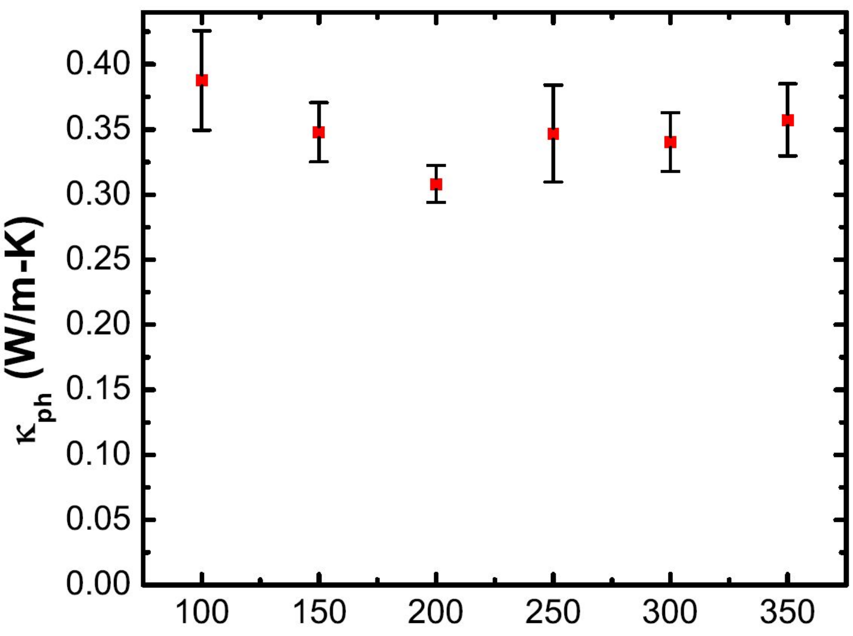


Fig. 4

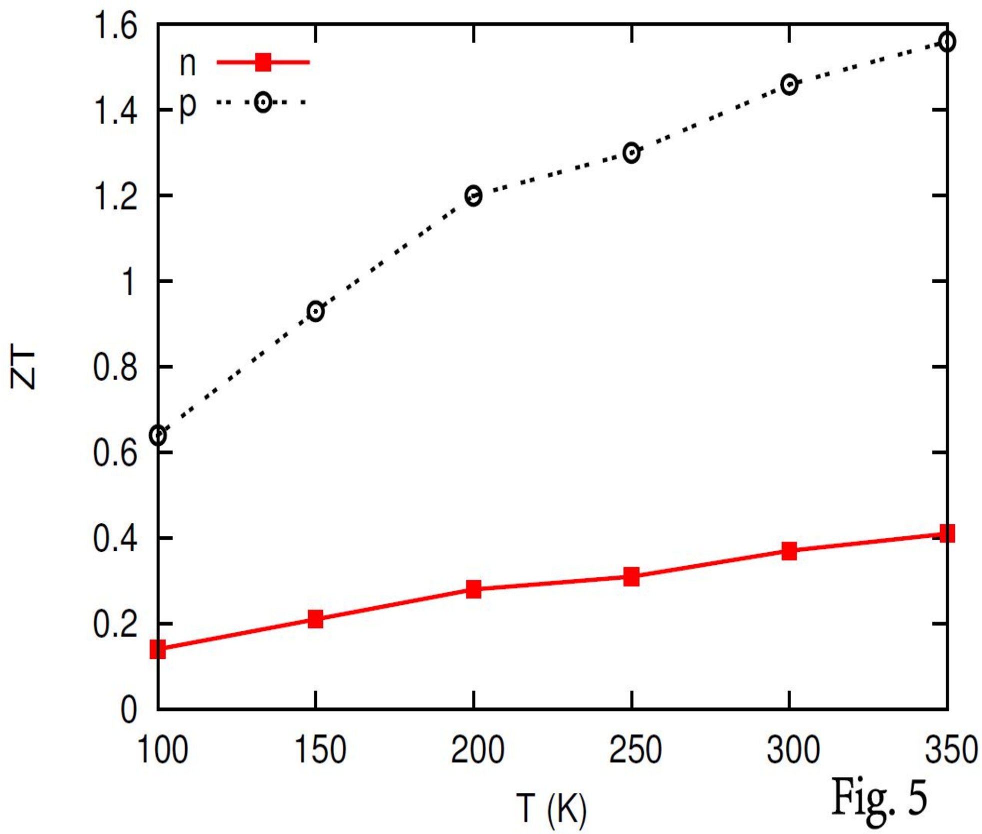


Fig. 5

Thermoelectric Performance of BDT

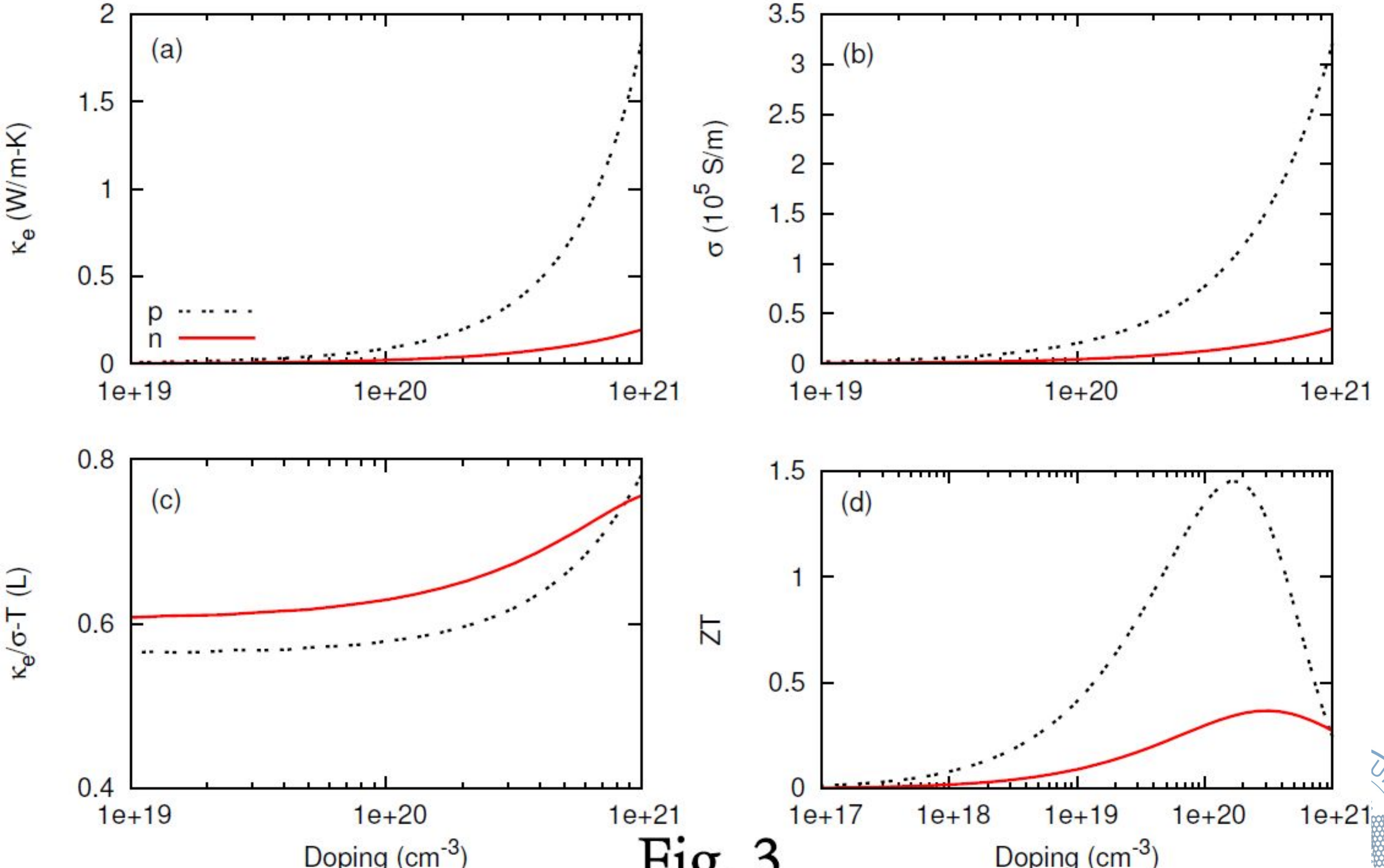


Fig. 3

Using the Bardeen-Shockley deformation potential theory,[6] the k-dependent relaxation time is[7]

$$\frac{1}{\tau(k)} \approx \frac{k_B T D^2}{\hbar^2 C |v_k|}. \tag{S4}$$

Here, D is the deformation potential, C is the elastic constant, k_B is the Boltzmann constant.

•总结 Conclusions

•1D: 纳米管聚乙烯链高热导率

•2D: 石墨烯圆盘梯度热导率

- •11.1/16:00空中乐园P377,安盟

•2D: 单层二硫化钼热电属性

- •11.1/15:15地球村，廖全文
- •11.1/16:00空中乐园P368,金泽林

•3D: 分子晶体热电新思路

- •10.31/15:30地球村，余晓翔
- •11.1/16:00空中乐园P342,丁鸿儒

•1D: CNT-PE array

- •High κ

•2D: Graphene Nano-disk

- •Graded κ (r)

•2D: MoS2

- •TE Performance

•3D: Molecular crystals

- •TE Performance

•Thanks for co-authors

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- Doctors L.Yang @NUS

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