Enhancing the Figure-of-Merit in Half-Heuslers for Vehicle Waste Heat Recovery

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Outline

- Why Half-Heuslers for auto waste heat recovery?
- Status of Half-Heuslers before our work
- The effect of nanostructures on thermoelectric figure-of-merit
- The effect of larger differences in atomic mass and size on thermal conductivity and thermoelectric figure-of-merit

- Bonus: New promising materials with good ZT

Why Half-Heuslers?

Compounds		Bi_2Te_3	PbTe/PbSe	Skutterudites	Half-Heusler	SiGe
Working Temperature		-100-200 °C	100-500 °C	100-500 °C	100-700 °C	100-1000 °C
Peak ZT	N	1.1	1.3	1.7	1.1	1.3
	P	1.4	1.8	1.0	1.1	1.0
Supply		Te	Te	Rare-earth		Ge
Cost		moderate	moderate	low	moderate	high
Toxicity		low	high	low	low	low
Mechanical Strength		moderate	poor	moderate	high	high
Thermal Stability		moderate	poor	poor	high	high
Contact		easy	done	being studied	easy	done

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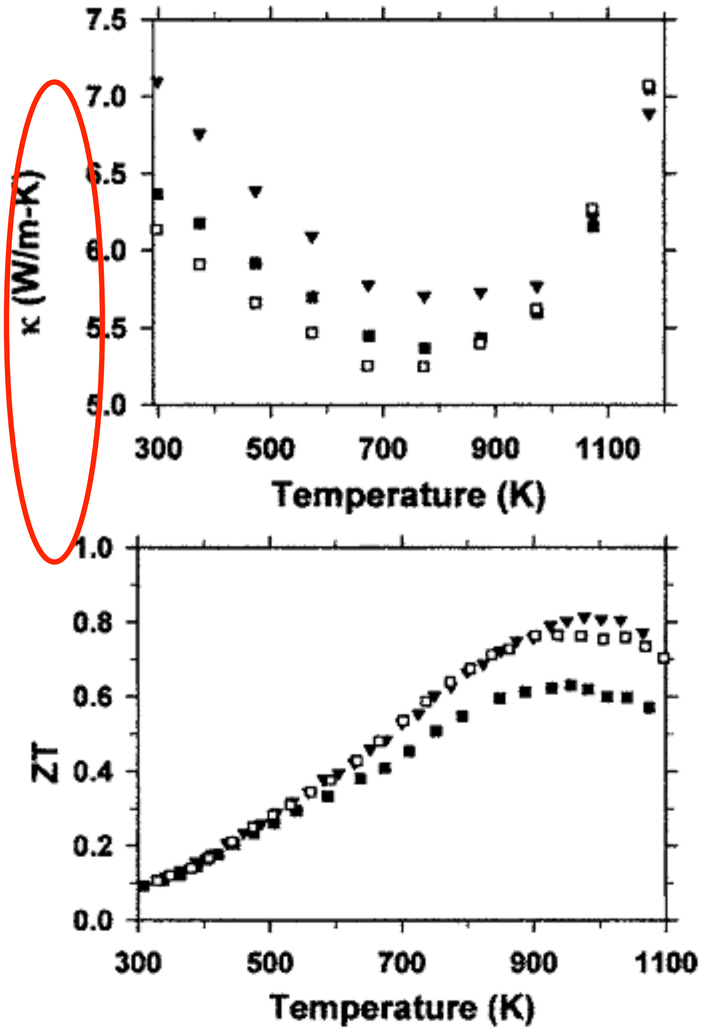
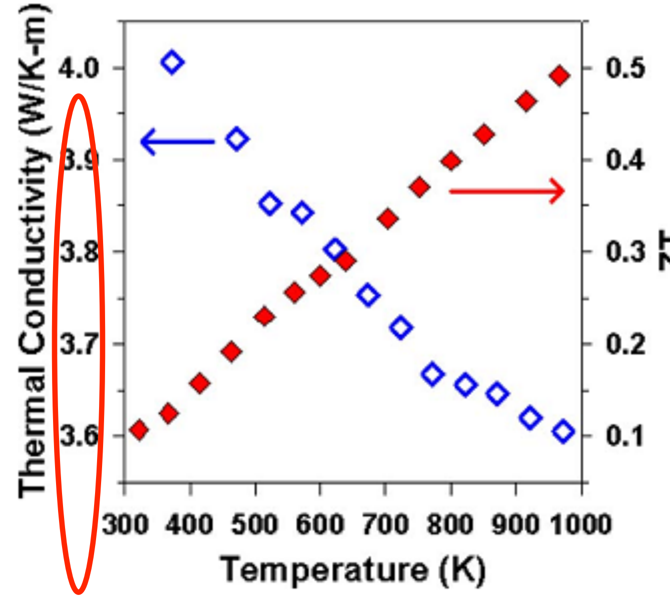
Status of Half-Heuslers

N type, $Hf_{0.75}Zr_{0.25}NiSn_{0.975}Sb_{0.025}$



Culp et al., *Appl. Phys. Lett.* **88**, 042106 (2006)

P type, $Zr_{0.5}Hf_{0.5}CoSb_{0.8}Sn_{0.2}$



Culp et al., *Appl. Phys. Lett.* **93**, 022105 (2008)

- Thermal conductivity too high!
- Nanocomposite approach: reduce thermal conductivity

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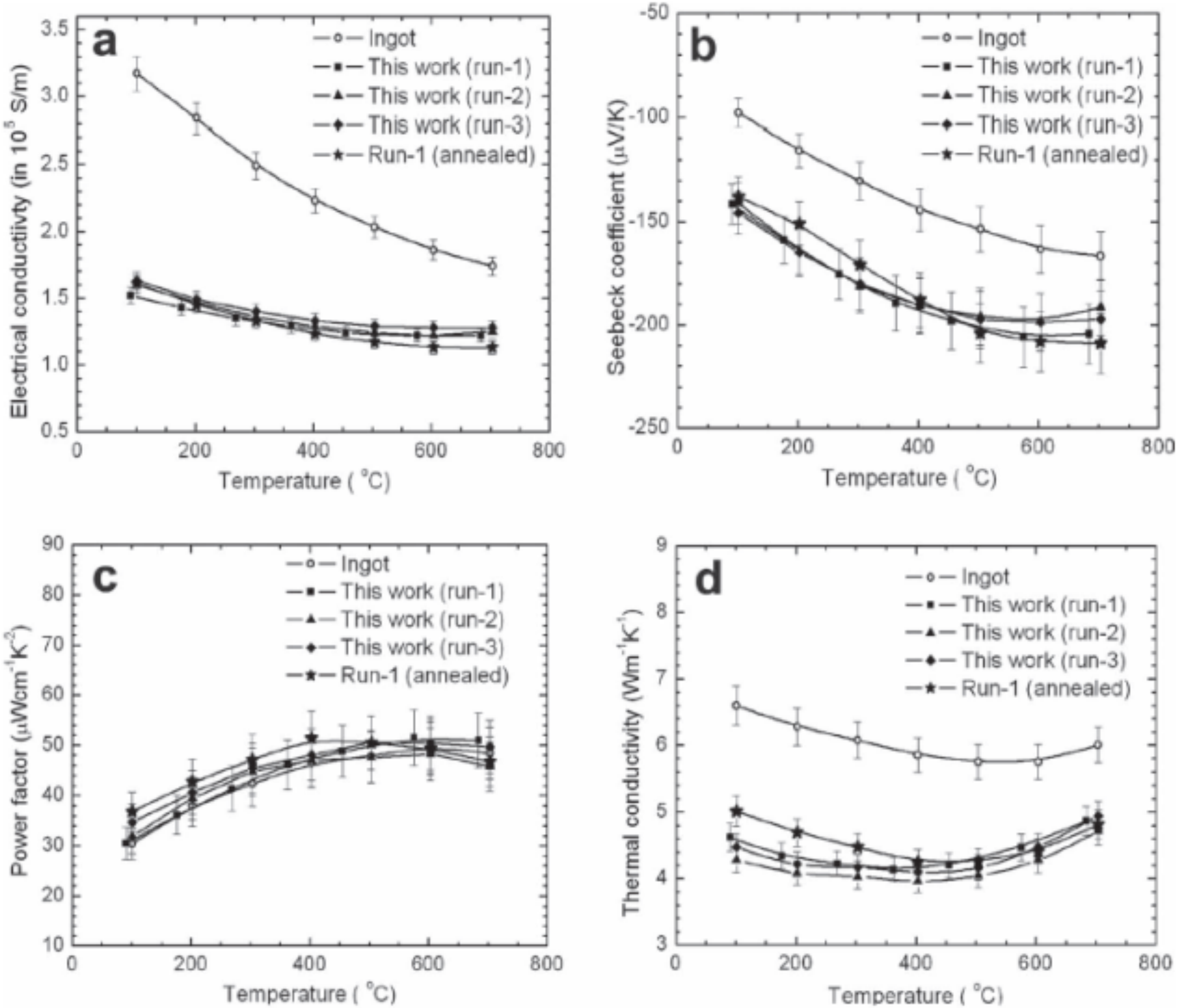
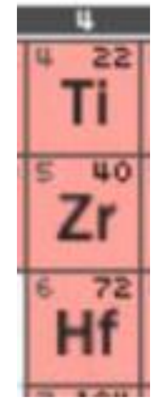
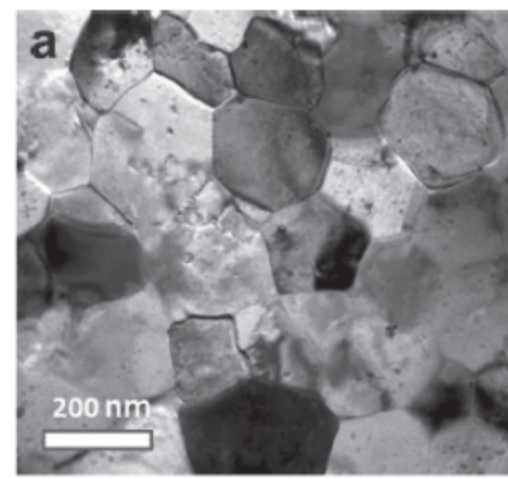
Phonon Engineering nanostructure in n-type half-Heusler

Giri Joshi, *Adv. Energy Mater.* **2011**, *1*, 643–647

$Hf_{0.75}Zr_{0.25}NiSn_{0.99}Sb_{0.01}$

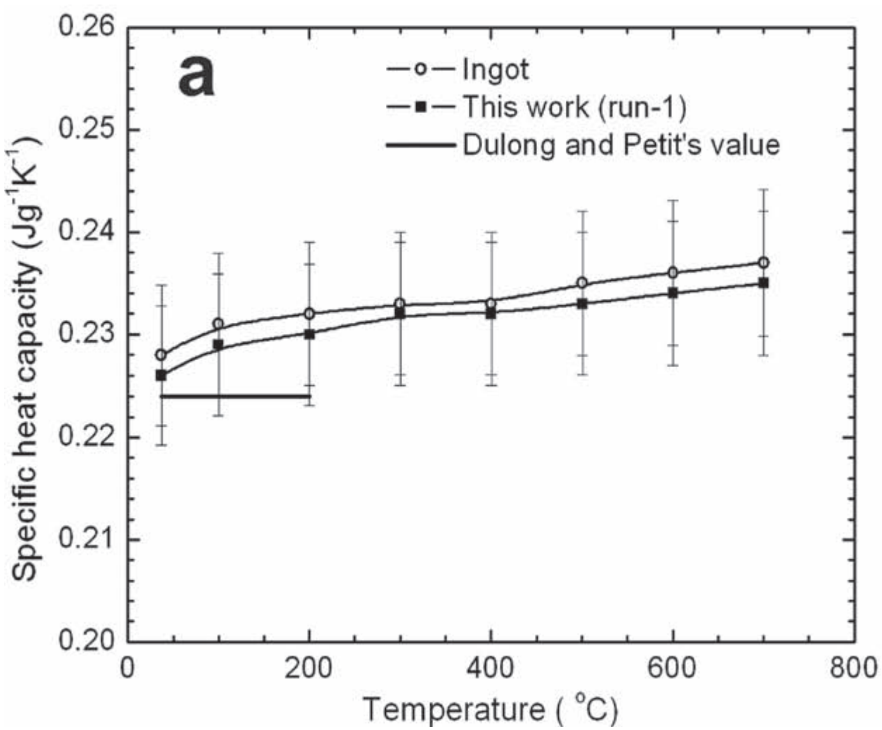


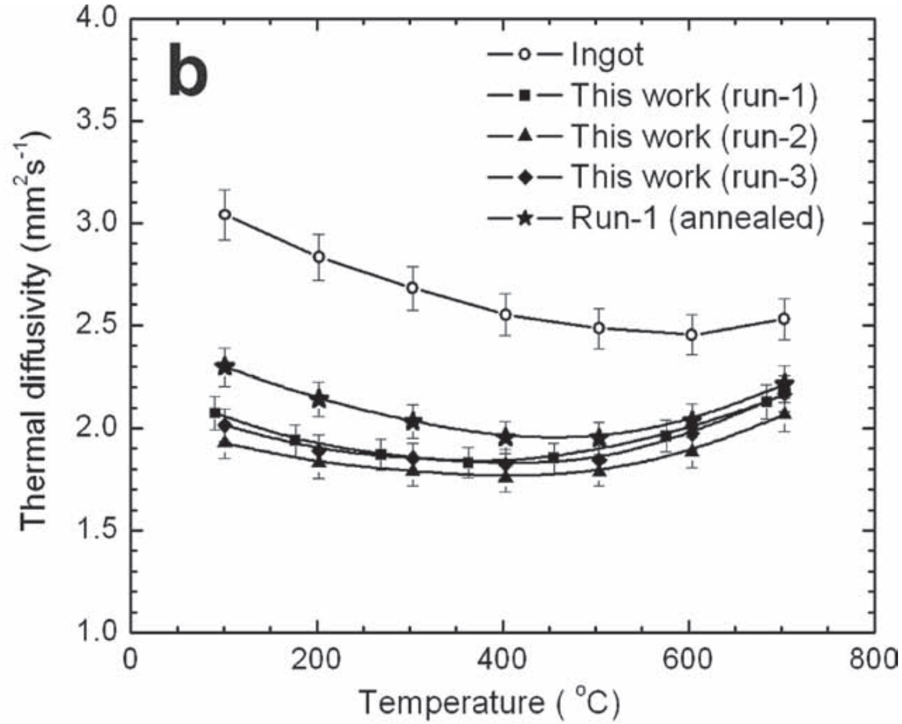




Specific heat and thermal diffusivity

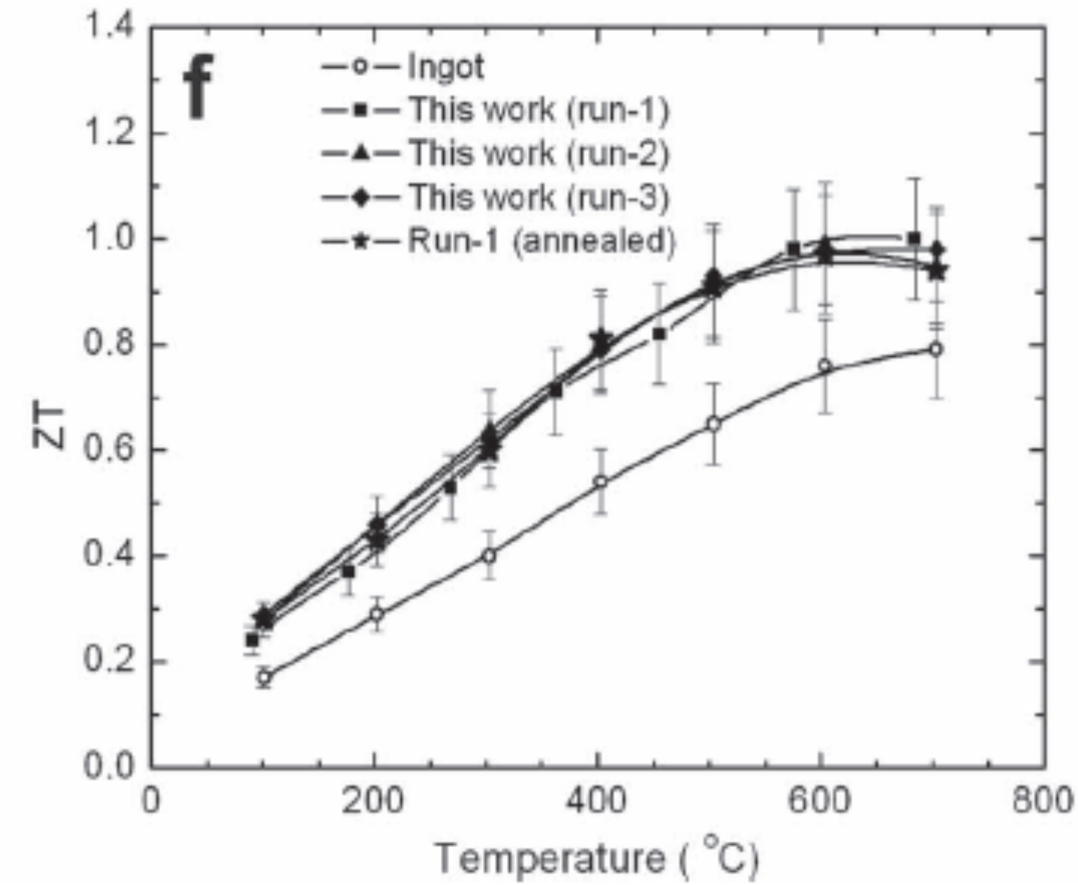
Giri Joshi, *Adv. Energy Mater.* **2011**, *1*, 643–647 $Hf_{0.75}Zr_{0.25}NiSn_{0.99}Sb_{0.01}$





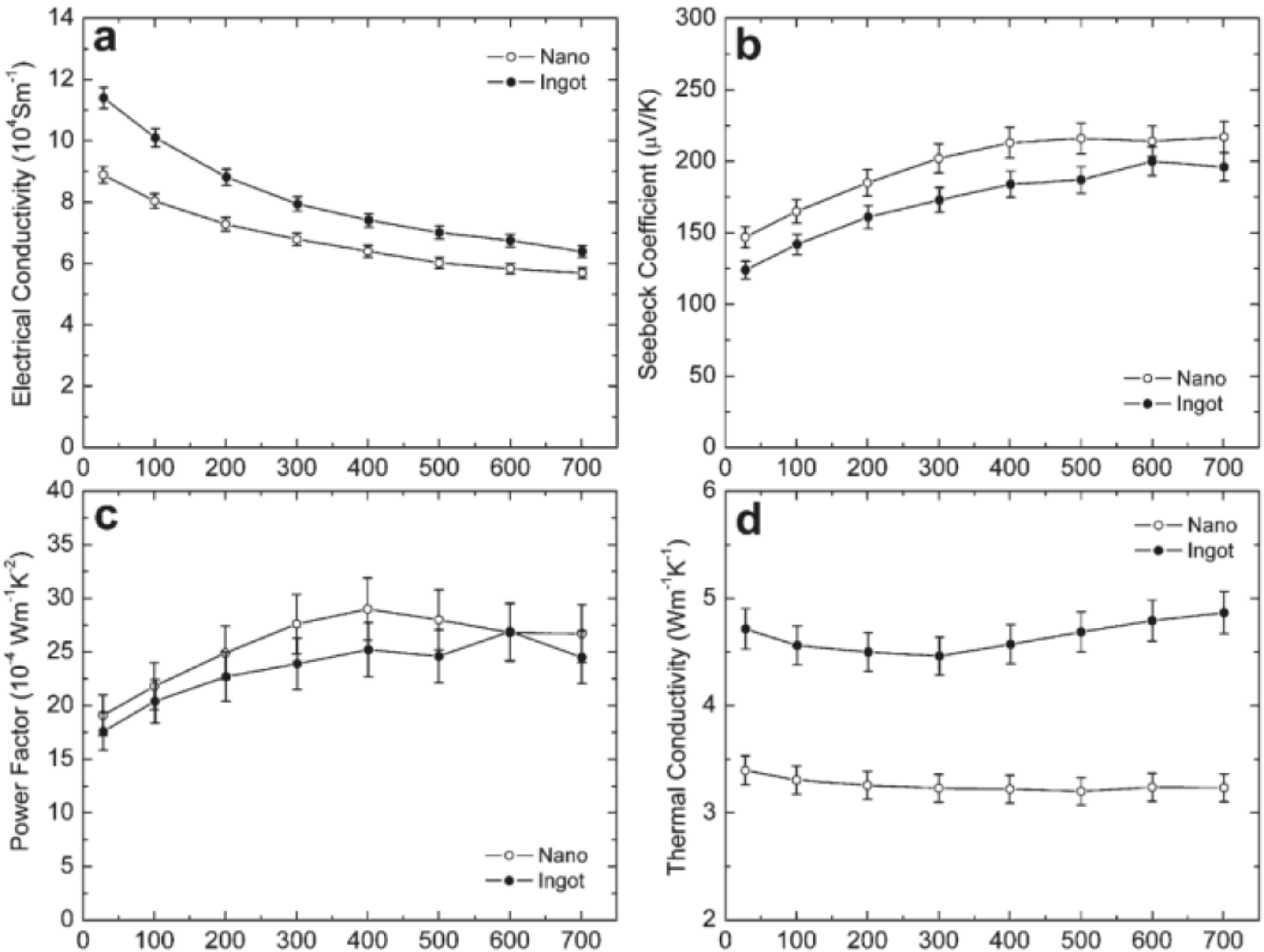
ZT Improvement due to Lower Thermal Conductivity by Nanostructures in n-type

Giri Joshi, *Adv. Energy Mater.* **2011**, *1*, 643–647 $Hf_{0.75}Zr_{0.25}NiSn_{0.99}Sb_{0.01}$



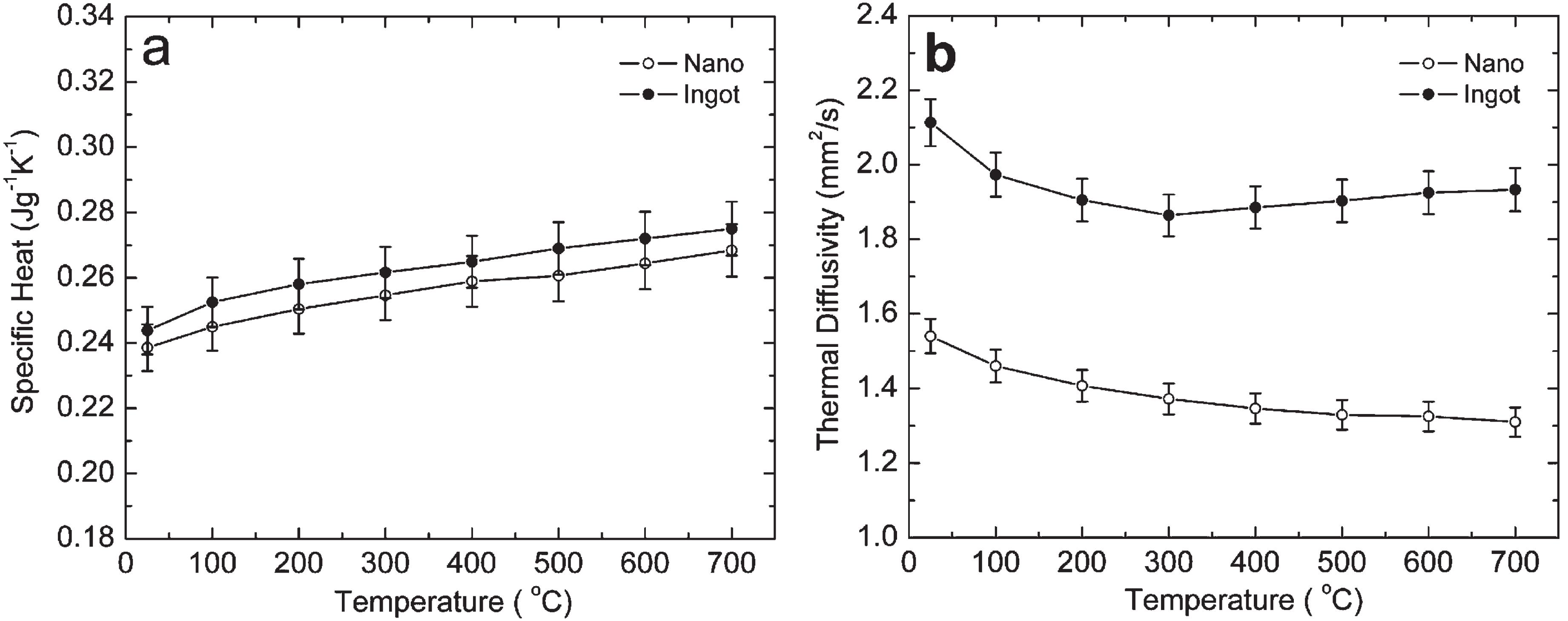
Effect of Nanostructures on p-type

Xiao Yan, *et al.*, *Nano Letters* **11**, 556-560 (2011)



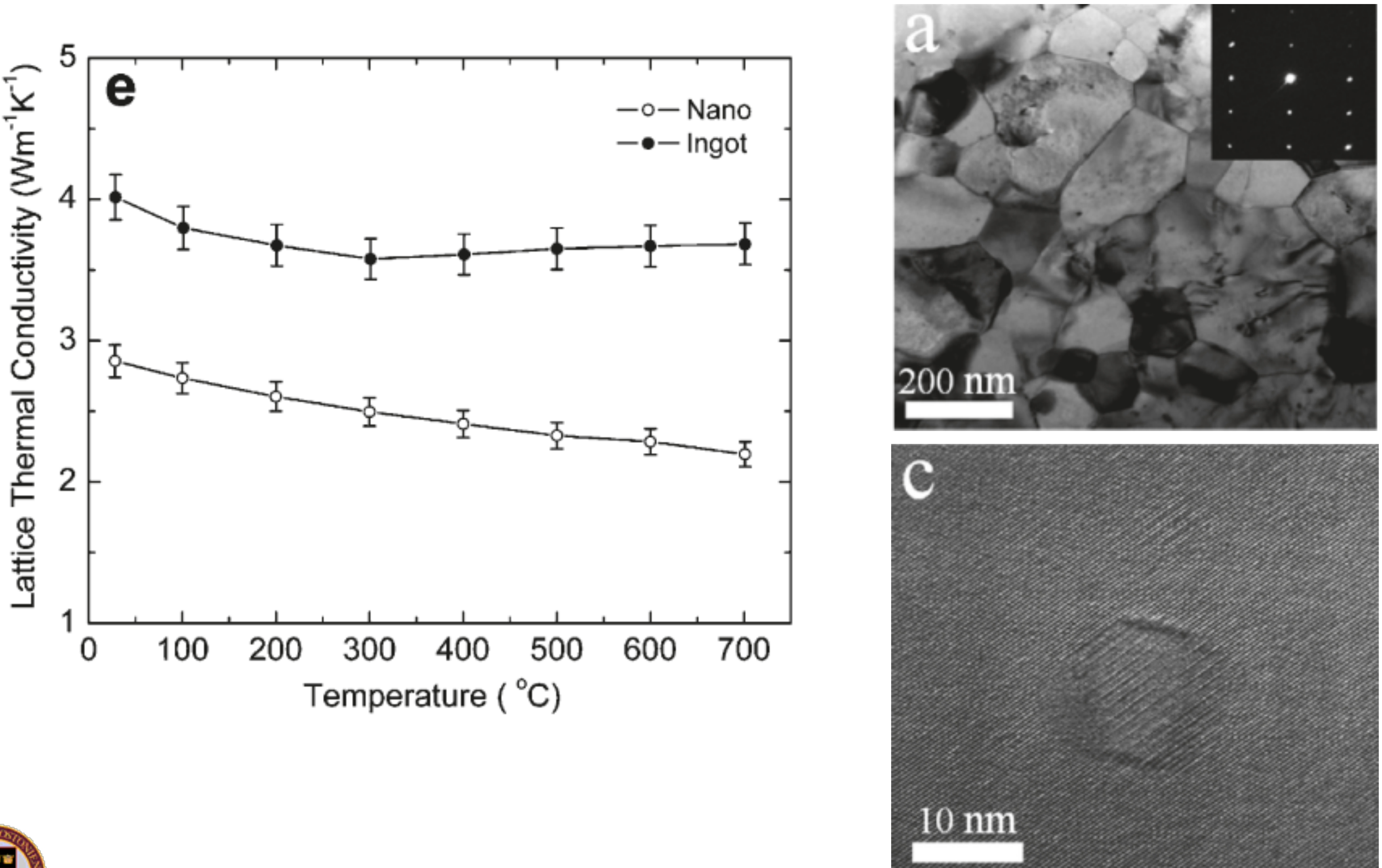
Specific heat and thermal diffusivity

Xiao Yan, *et al.*, *Nano Letters* **11**, 556-560 (2011)



Lattice thermal conductivity and nanostructures

Xiao Yan, *et al.*, *Nano Letters* **11**, 556-560 (2011)



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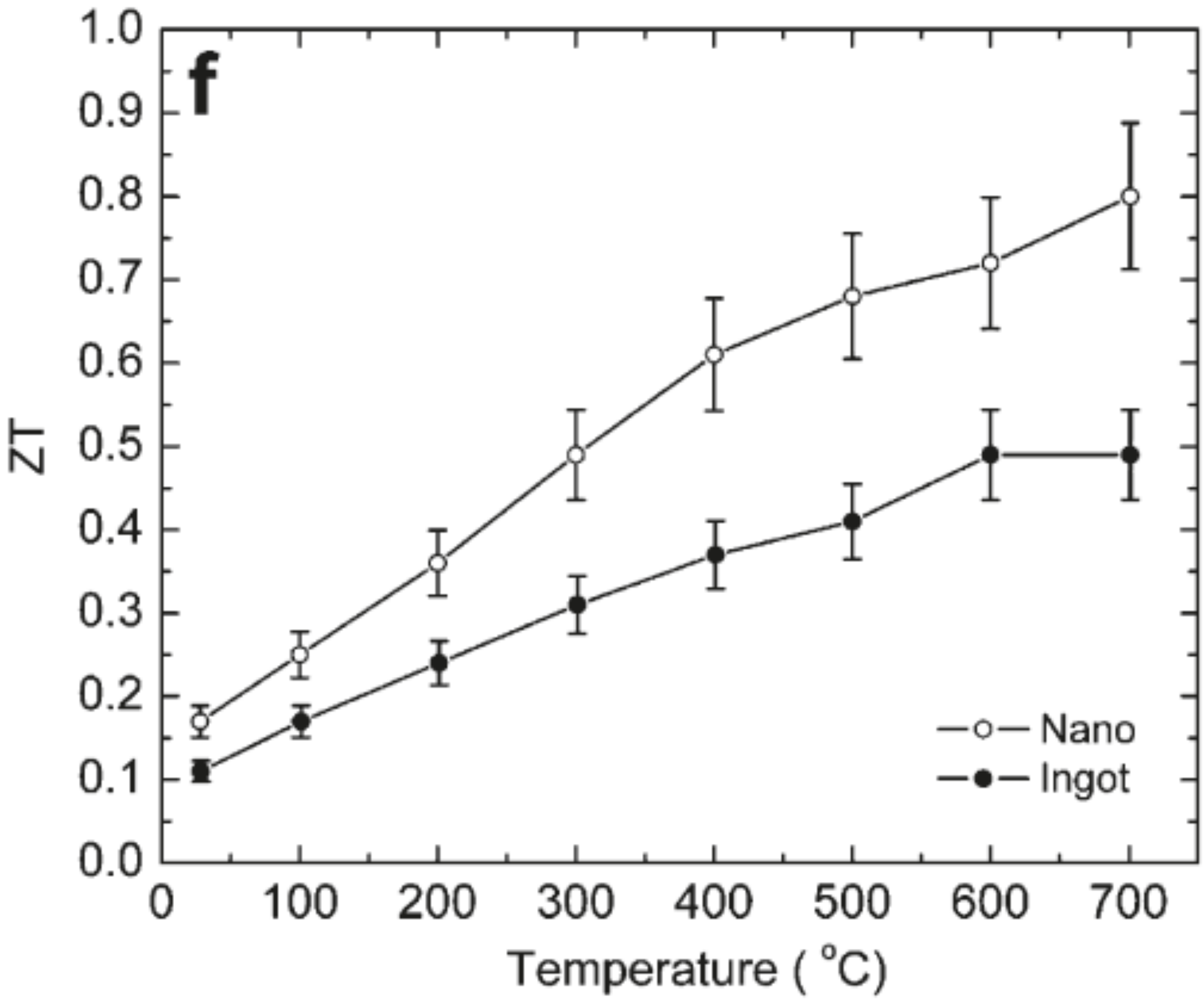
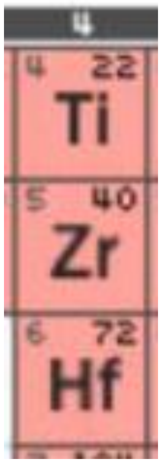
Improved ZT by Nanostructures in p-type Half-Heuslers

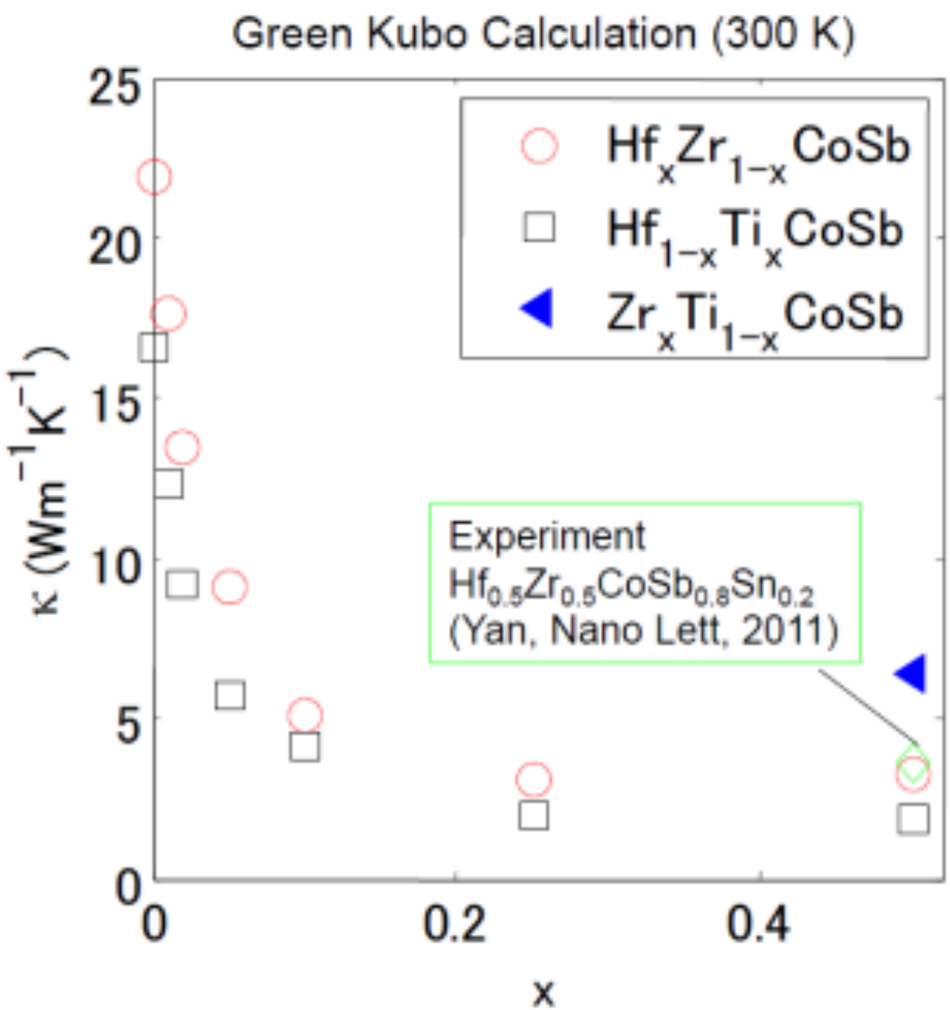
Xiao Yan, *et al.*, *Nano Letters* **11**, 556-560 (2011)



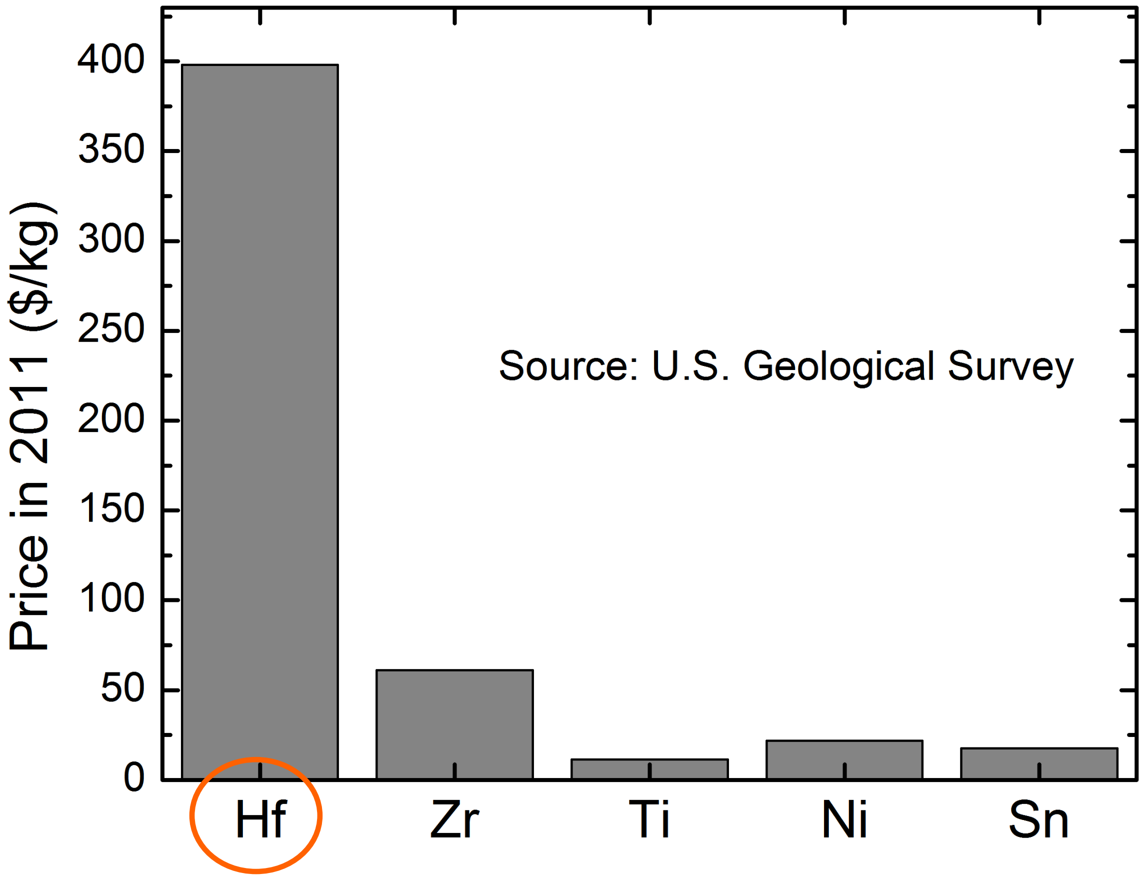
Phonon Engineering larger differences in mass and size in half-Heuslers

Shiomi, Esfarjani, Chen, Phys. Rev. B 84, 104302 (2011)



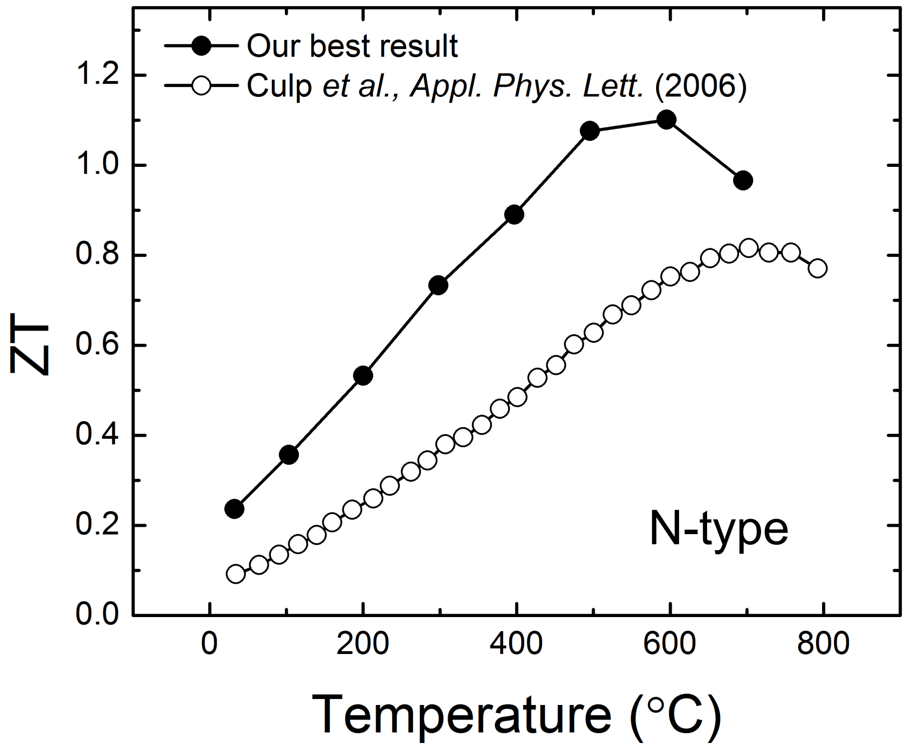


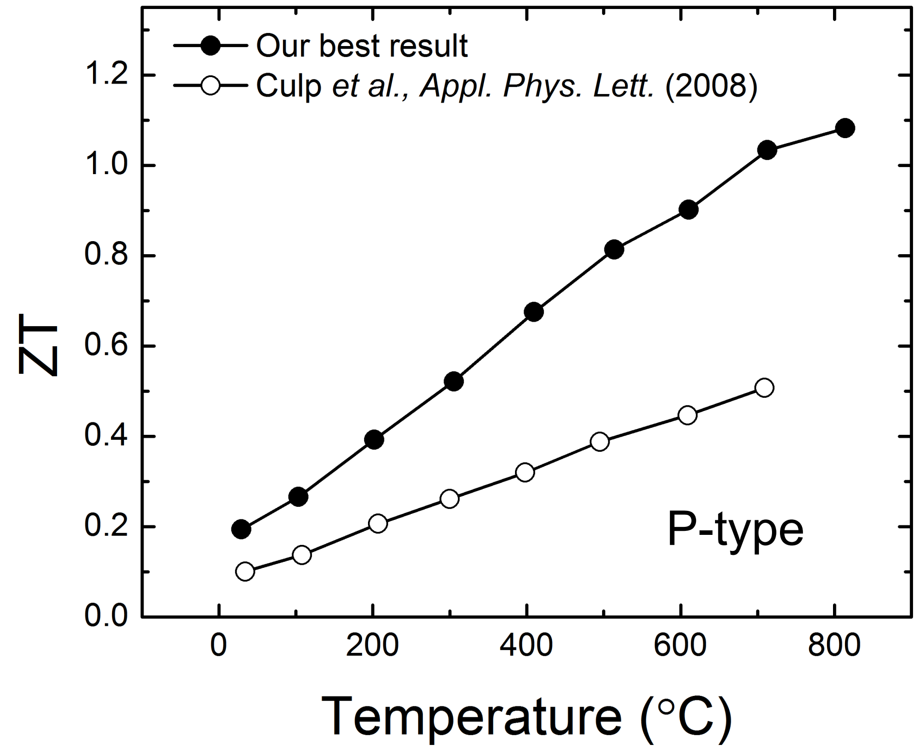
How to Further Cut the Cost?



Need to reduce the usage of Hf as much as possible.

Summary for Half-Heuslers



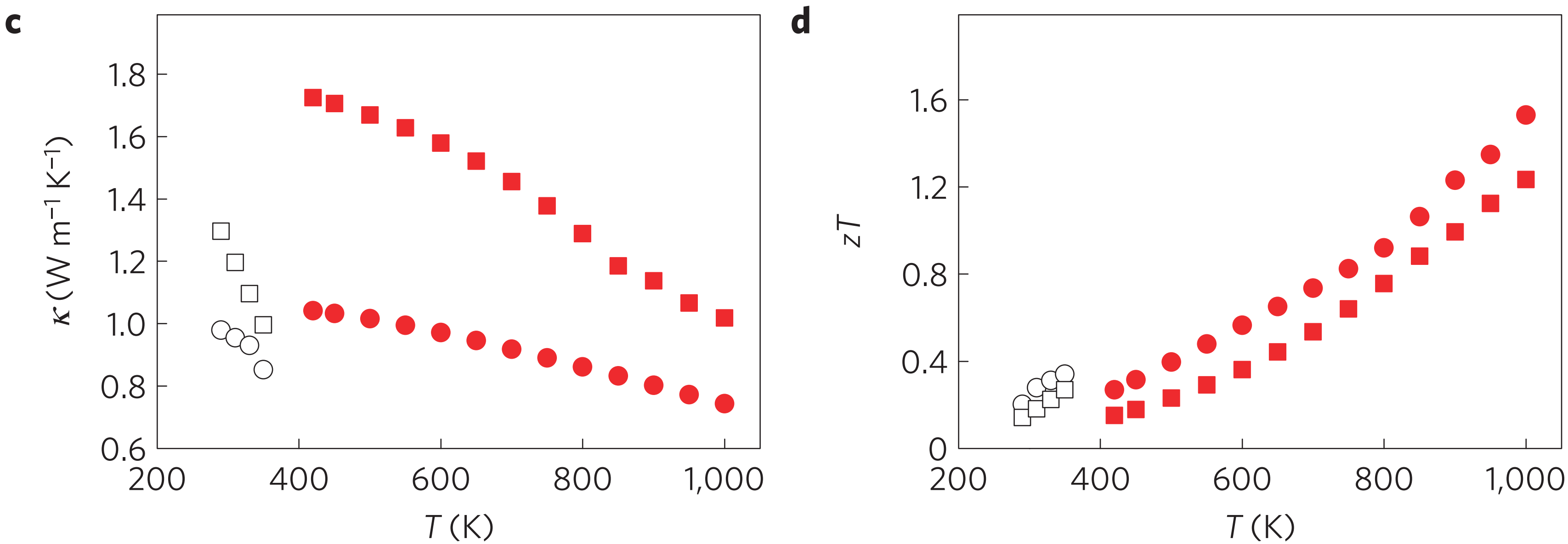


A New Potentially Interesting TE Material: Cu_2Se

Copper ion liquid-like thermoelectrics

Huili Liu[1,2], Xun Shi[1,3]★, Fangfang Xu[3], Linlin Zhang[3], Wenqing Zhang[3], Lidong Chen[1]★, Qiang Li[4], Ctirad Uher[5], Tristan Day[6] and G. Jeffrey Snyder[6]

NATURE MATERIALS DOI: 10.1038/NMAT3273



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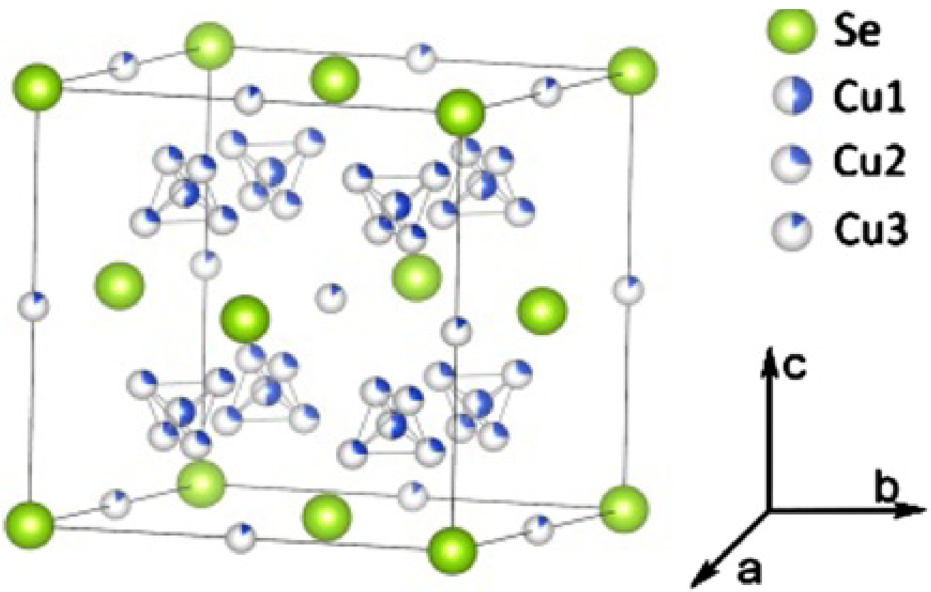
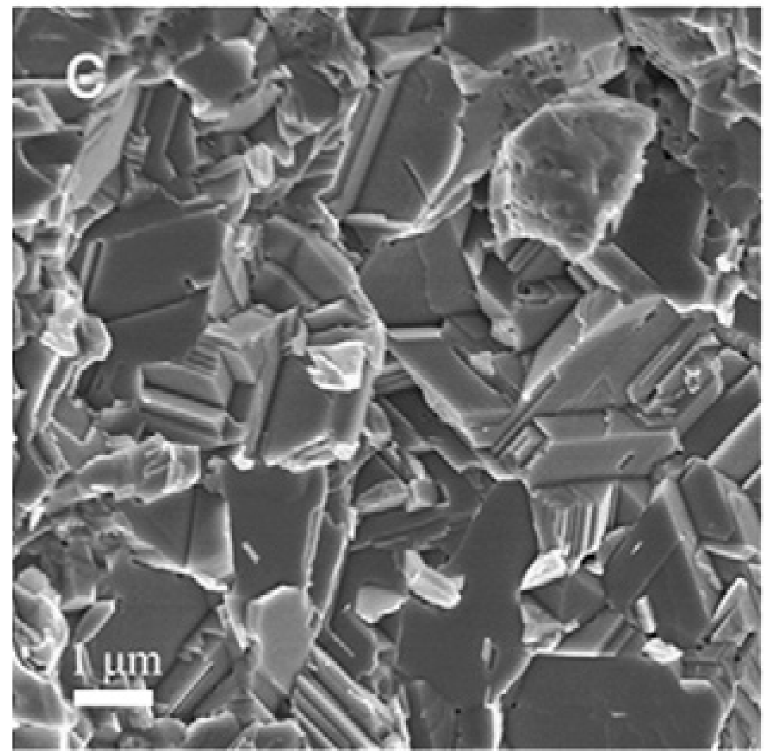
Thermoelectric properties of copper selenide with ordered selenium layer and disordered copper layer

Bo Yu[a,1], Weishu Liu[a,1], Shuo Chen[a], Hui Wang[a], Hengzhi Wang[a], Gang Chen[b,*], Zhifeng Ren[a,*]

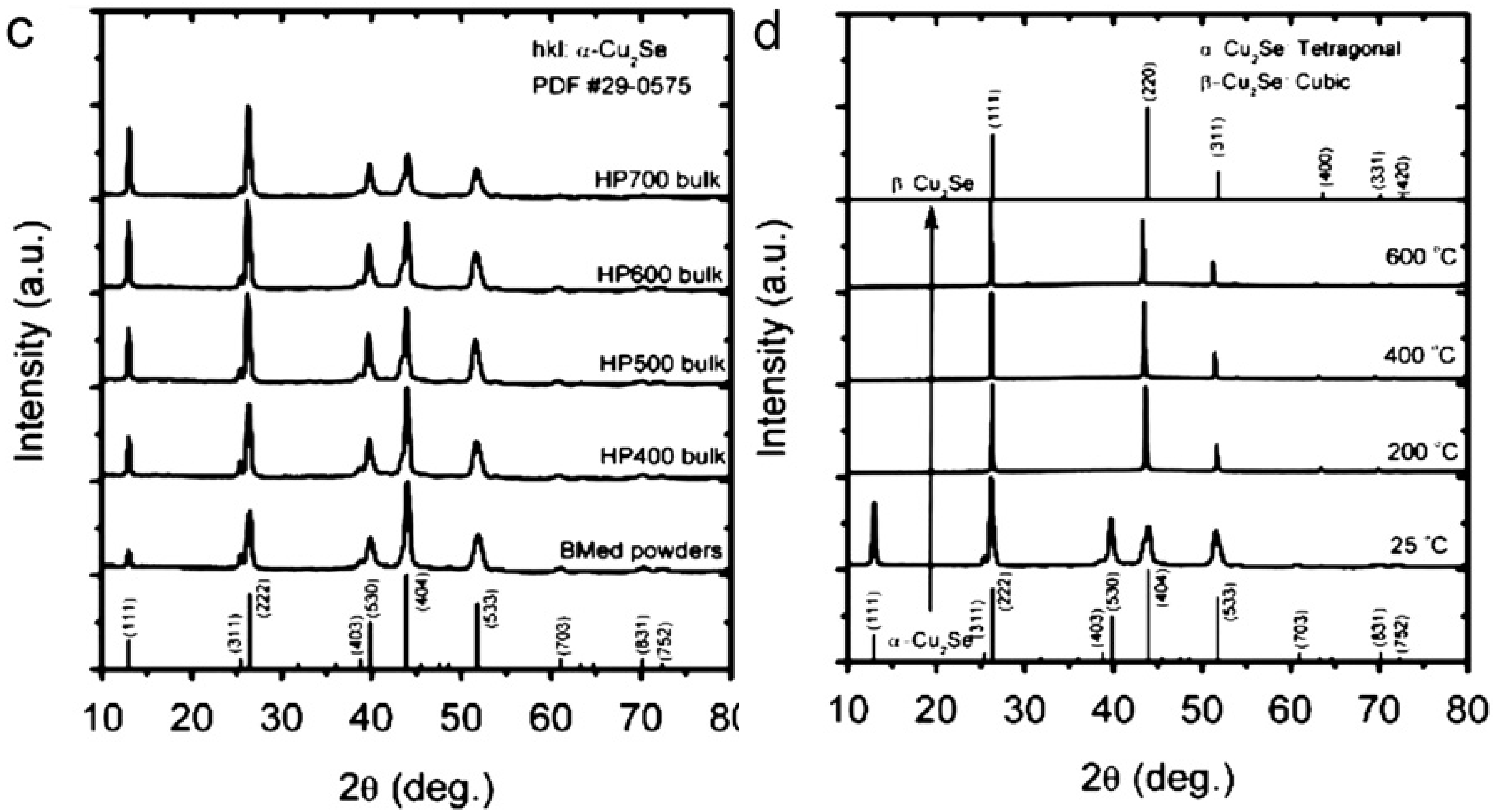
Nano Energy (2012), doi:10.1016/j.nanoen.2012.02.010





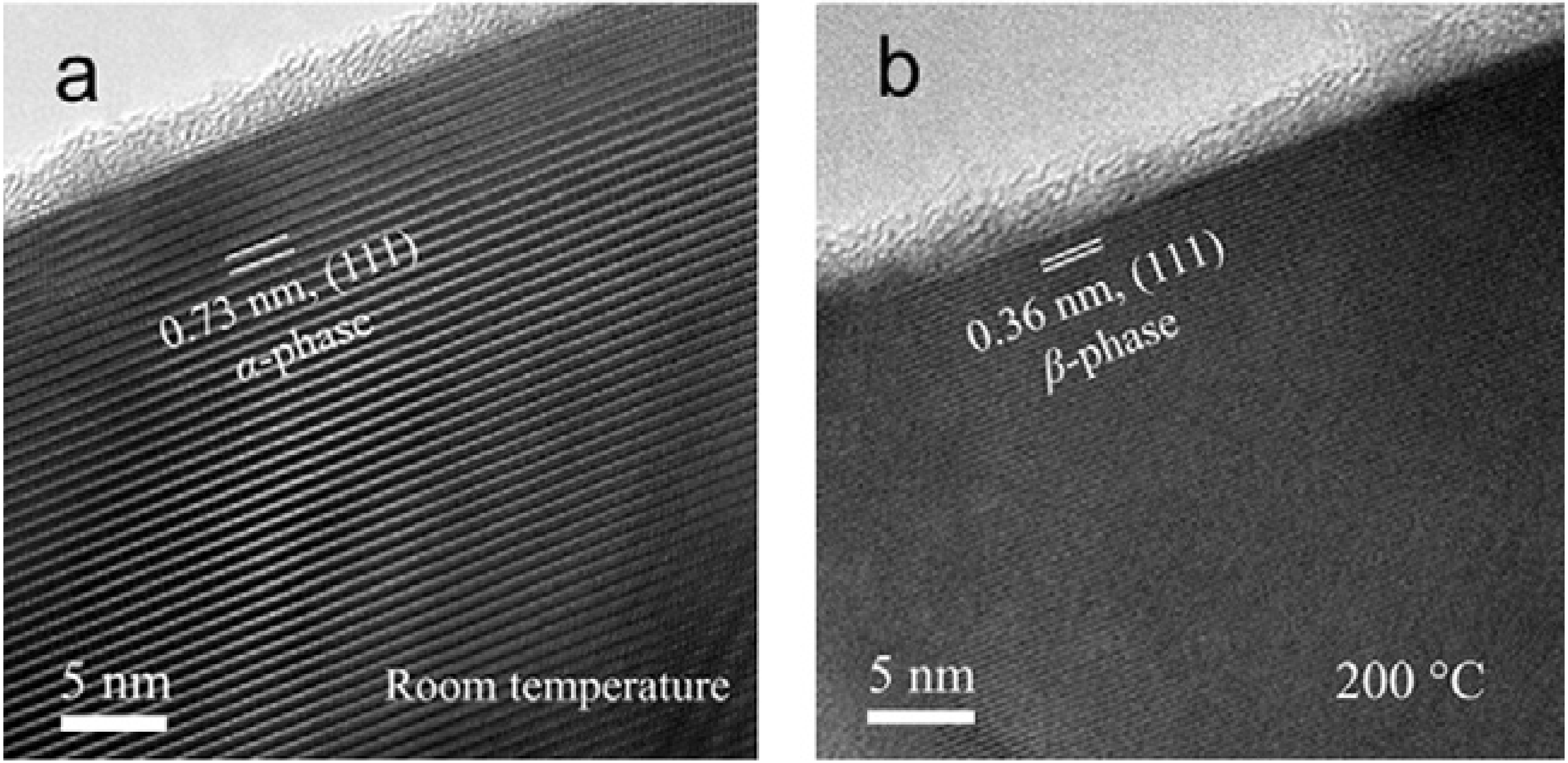
Effect of pressing temp. on structure of Cu_2Se

Nano Energy (2012), doi:10.1016/j.nanoen.2012.02.010



Structure change observed by TEM

Nano Energy (2012), doi:10.1016/j.nanoen.2012.02.010



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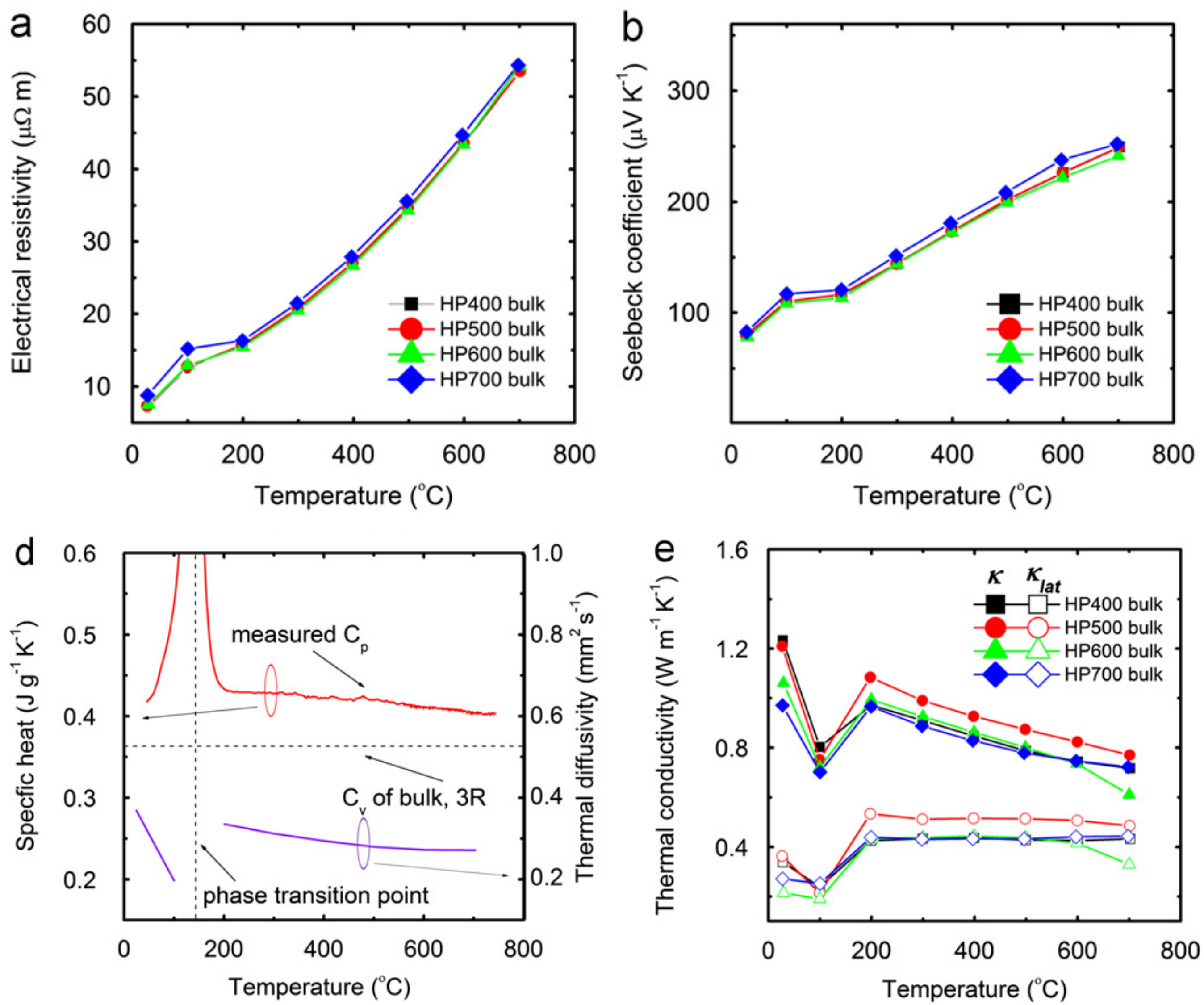
Thermoelectric properties of Cu_2Se

Nano Energy (2012), doi:10.1016/j.nanoen.2012.02.010



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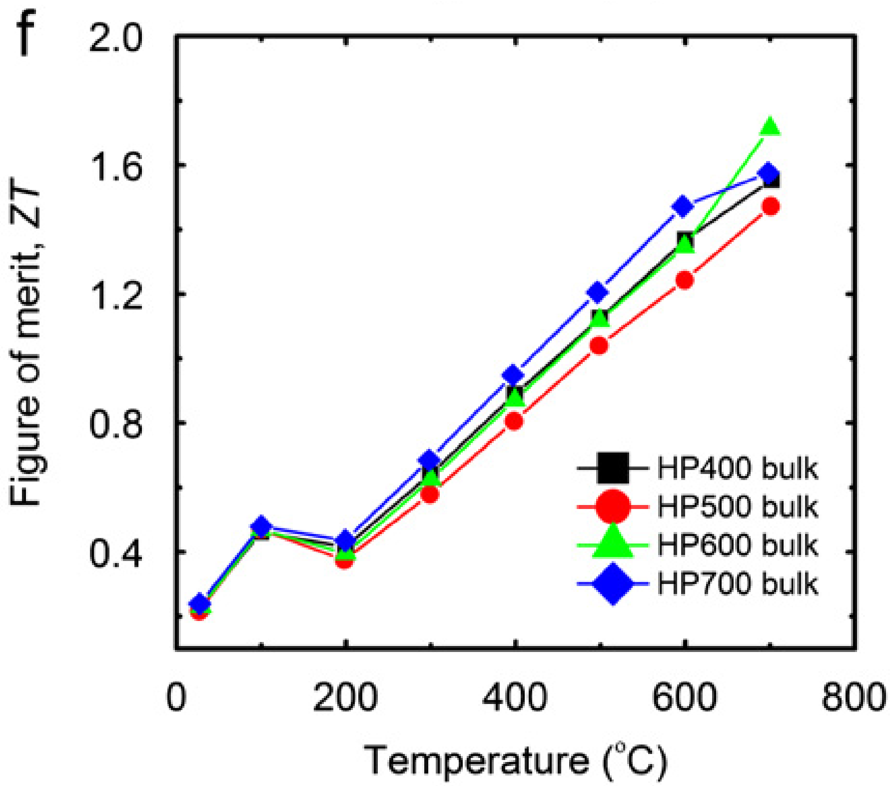
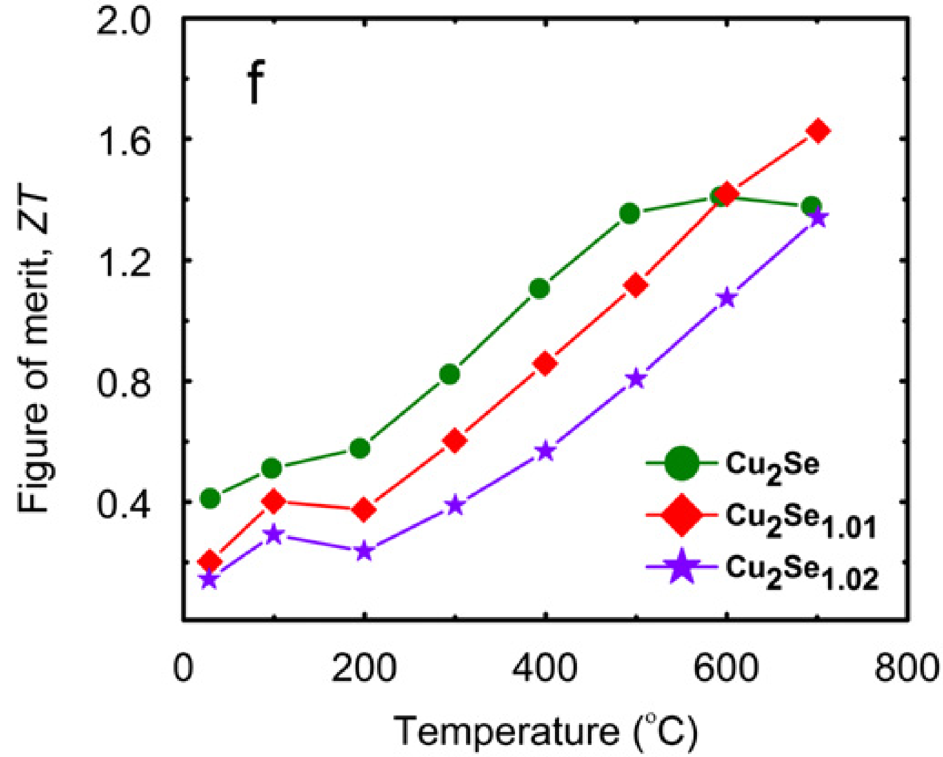
ZT vs. temperature of Cu_2Se

Nano Energy (2012), doi:10.1016/j.nanoen.2012.02.010





Summary for Cu_2Se

- Good ZT may happen in non traditional thermoelectric materials
- Structure with ordered layer for charger carrier and disordered layer for phonon scattering is probably a good way to get high ZT
- Search of ZT higher than 2 should be in a lot of exotic materials

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- Prof. Gang Chen at MIT