

# Precis of Workshop

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Properties and Applications of Thermoelectric Materials

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Figure of merit

$$ZT = \frac{TS^2\sigma}{\kappa}$$

dimensionless number

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## Properties and Applications of Thermoelectric Materials

“Review new materials and examine mechanisms that could lead to new thermoelectric and magnetocaloric devices with an enhanced figure of merit.”

$$ZT = \frac{TS^2\sigma}{\kappa}$$

Efficiency of any thermoelectric device depends on ZT and practical applications require  $ZT \sim 1$  or even better  $ZT > 1$

Aim:

$$ZT = \frac{TS^2\sigma}{\kappa} \sim 1$$

Success would mean

Generate power from waste heat -----use for example in diesel trucks

Refrigerators with non-moving parts, etc.

Justify the investment of governments and other bodies in funding

basic materials research

## Strategies for enhancing ZT

$$ZT = \frac{TS^2\sigma}{\kappa_{\text{el}}} \frac{\kappa_{\text{el}}}{(\kappa_{\text{el}} + \kappa_{\text{latt}})}$$

Electronic figure of merit



Term involving  $\kappa_{\text{latt}}$ ,

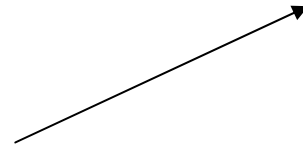


$< 1$

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Increase electronic factor



Reduce  $\kappa_{\text{latt}}$ .



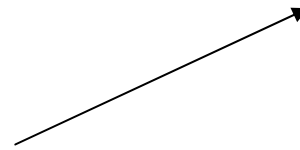
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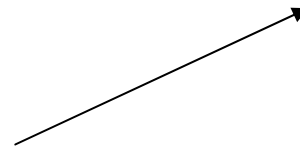
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Complex compounds with cages and rattlers that effectively scatter the phonons carrying the heat current

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Skutterudites, clathrates etc extensively reviewed by Takabatake, Maple, Rogl, and Bauer

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### Problem:

Good metals: large  $\sigma$  but low S

Insulators: large S but negligible  $\sigma$

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↓  
Strongly correlated Electron systems

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Metallic conductivity with large values of S

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Theoretical approaches using model Hamiltonians:

Vicinity of Mott transition (Kotliar)  
Mott transition with disorder (Kotliar)  
Vicinity of a Kondo insulator (Czcholl)

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First Principles calculations for specific materials

LDA +DMFT for a strongly correlated system (Held)

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Correlated Nanoscale multilayers designed to enhance thermoelectric response (Freericks)

Nanocomposites and systems with embedded with nanocrystals to block thermal transport (Sales)

Metallic glasses (Goncalves)

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New results using Thallium to increase the slope in DOS states at Fermi surface “valence skipper” --- +1 - +3 states seem to be involved (Sales)

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Future Perspective?

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## Future Perspective?

Clearly lots of ideas and encouraging results to keep everyone busy for the next few years

Lots of stimulating discussion in the workshop ---- and a particularly gratifying is the interest of the theoreticians in the experiments and the experimentalists in what theory might have to say.

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Thank you all for your contributions !

# Another Figure of Merit

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One familiar to you all !



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Veljko

Thank you Veljko !!!

and all your support team !!!