# Precis of Workshop

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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 ~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

$$ZT = \frac{TS^2\sigma}{\kappa_{\mathrm{el}}} \frac{\kappa_{\mathrm{el}}}{(\kappa_{\mathrm{el}} + \kappa_{\mathrm{latt}})} < 1$$

Electronic figure of merit

Term involving $\kappa_{\mathrm{latt}}$

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

$< 1$

Increase electronic factor

Reduce $\kappa_{\mathrm{latt}}$

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

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Skutterrudites. clathrates etc extensively reviewed by Takabatake, Maple, Rogl,. and Bauer

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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  !!!