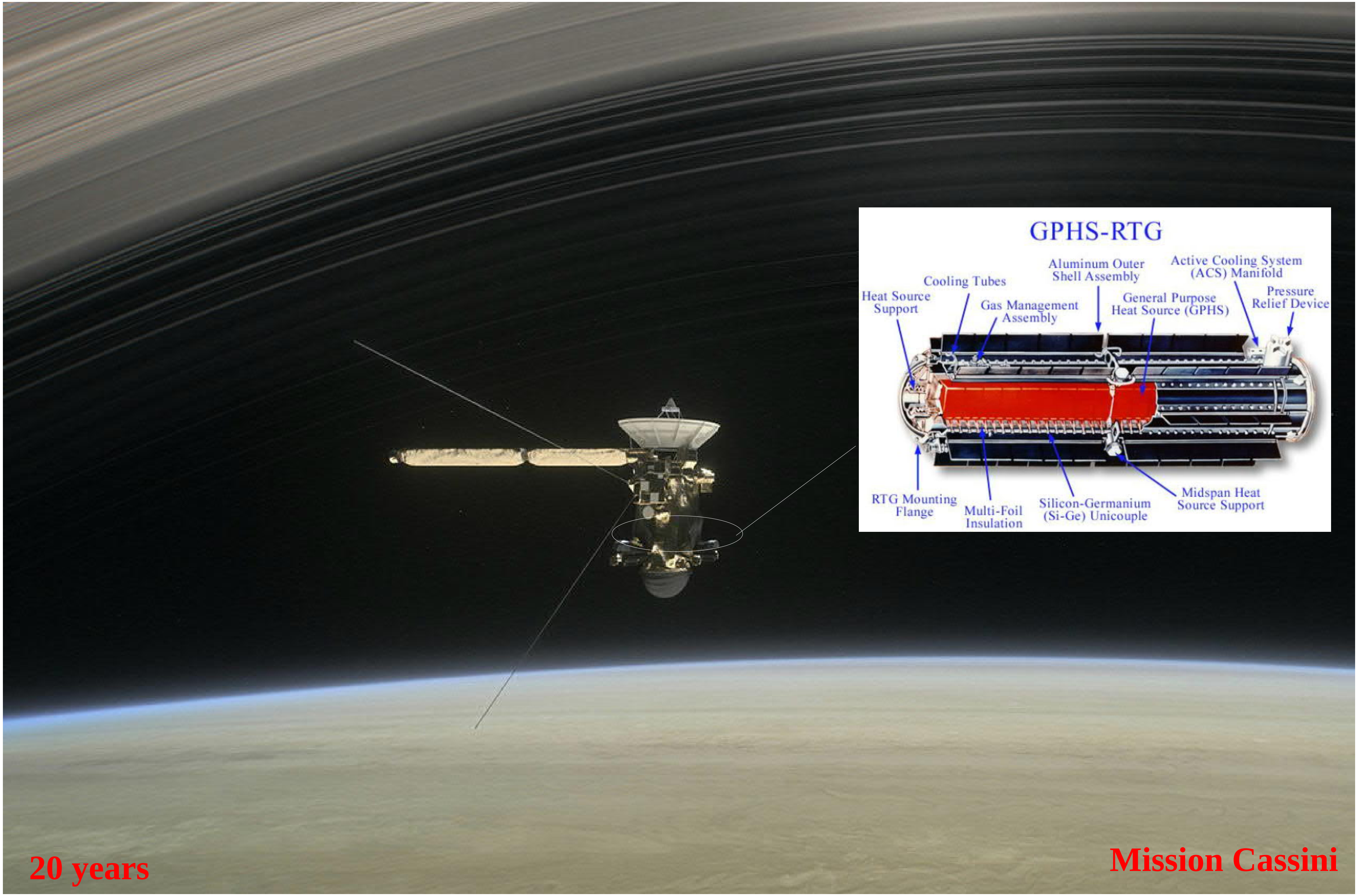

ЗА КРАЩУ
СТУДЕНТСЬКУ
НАУКОВУ РОБОТУ
1975 року

1975


НАЦІОНАЛЬНА АКАДЕМІЯ НАУК УКРАЇНИ

2019

Courtesy NASA/JPL-Caltech/Space Science Institute



https://solarsystem.nasa.gov/missions/cassini/mission/grand-finale/overview/ *Courtesy NASA/JPL-Caltech/Space Science Institute*

Thermoelectric materials

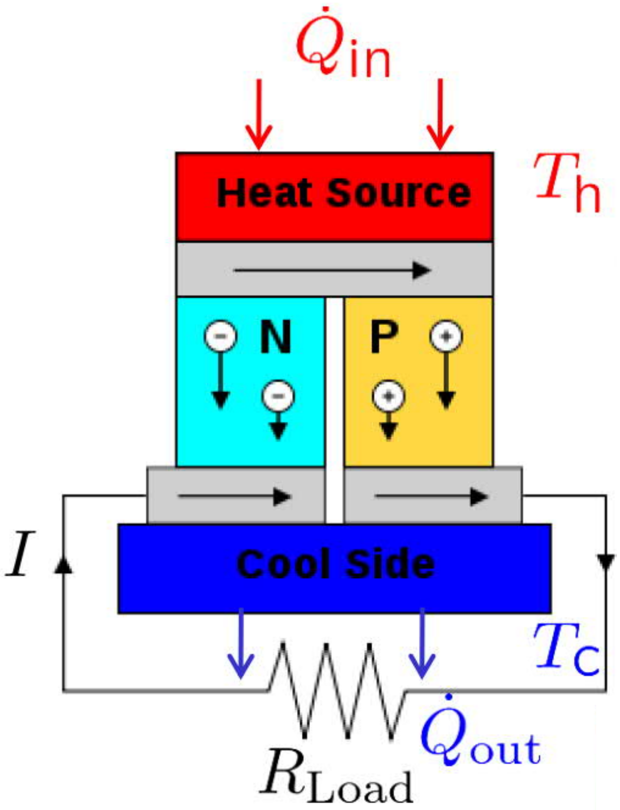
Термоелектричні матеріали

Yuri Grin

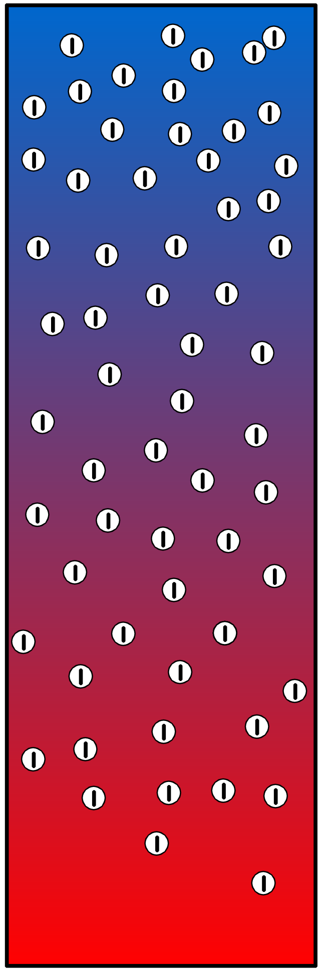
Max-Planck-Institut für Chemische Physik fester Stoffe Dresden

Courtesy NASA/JPL-Caltech/Space Science Institute

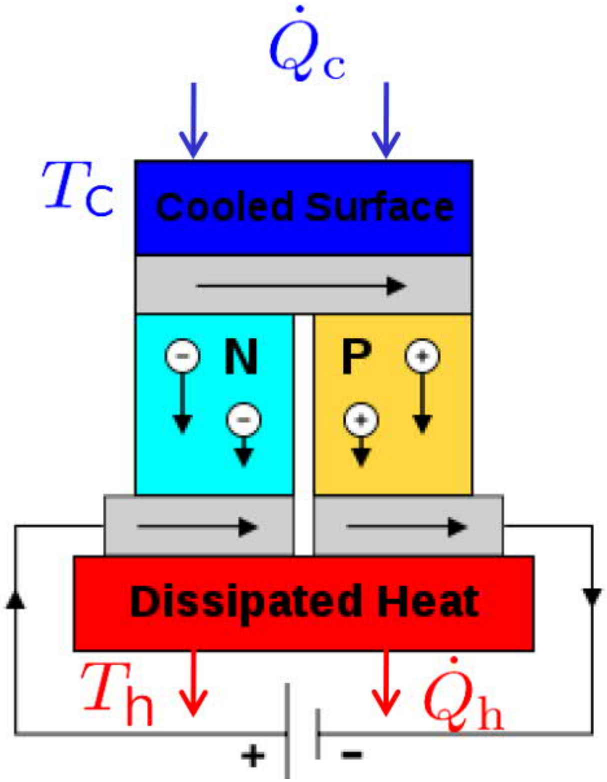
Seebeck effect *vs* Peltier effect



cold

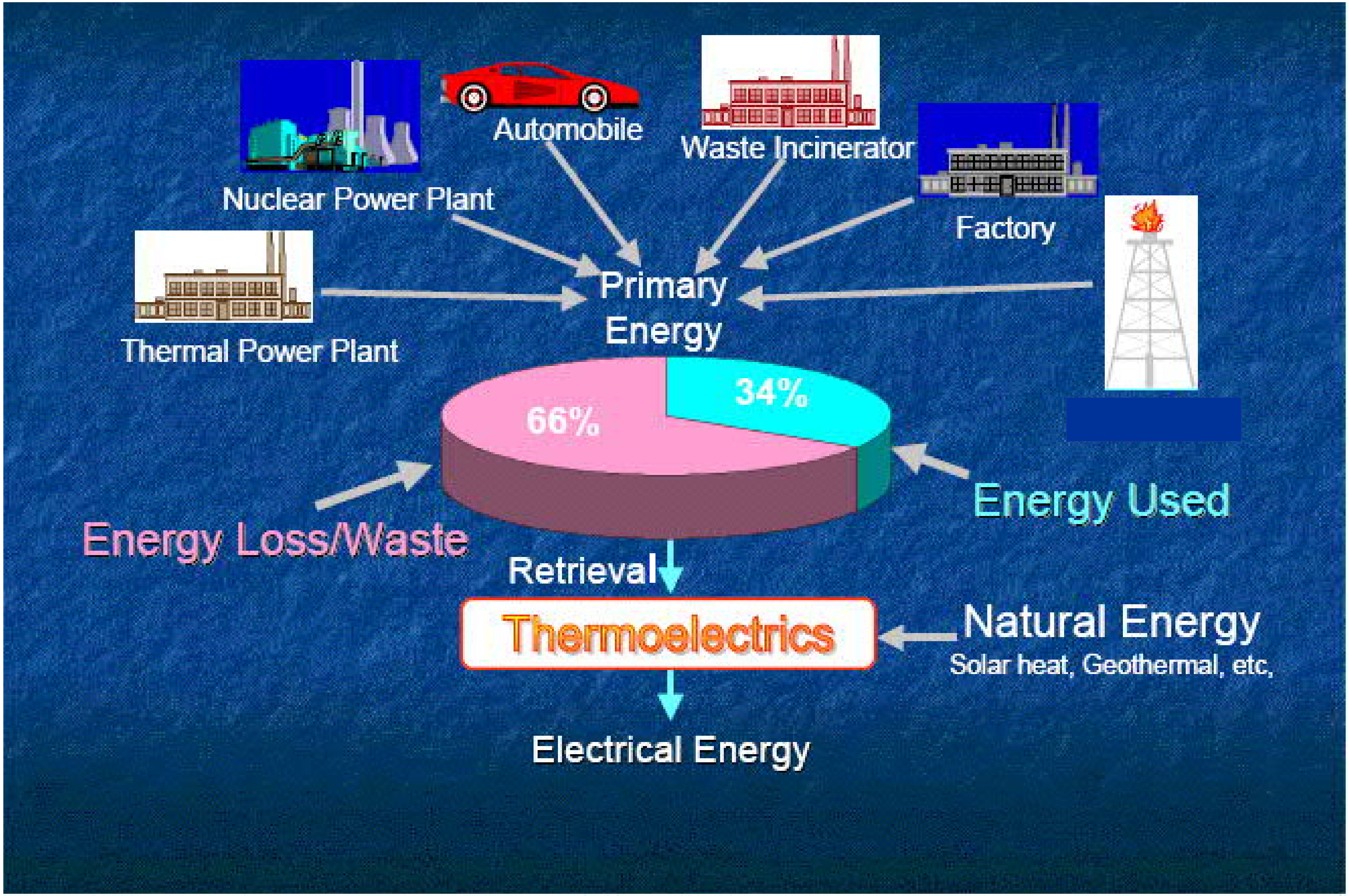


hot



G. J. Snyder, E. S. Toberer, Nature Materials 7 (2008) 105

Thermoelectrics for heat waste recycling



Thermoelectrics for heat waste recycling

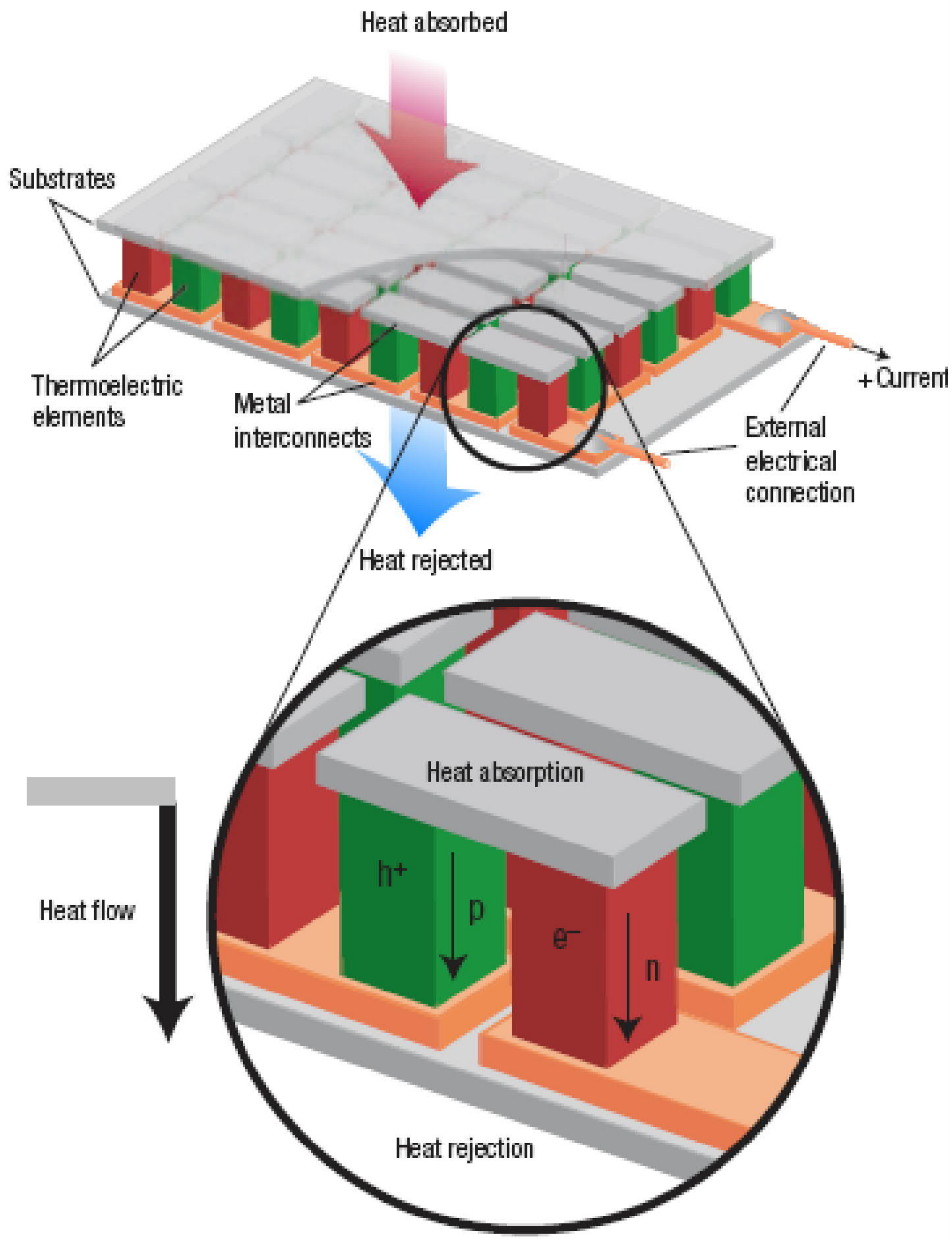
Тепер нам залишається лише перетворити тепло у електричний струм!!

Badische Zeitung, 30.06.2007; Courtesy Dr. H. Böttner

Thermoelectric generator

Thermoelectric module

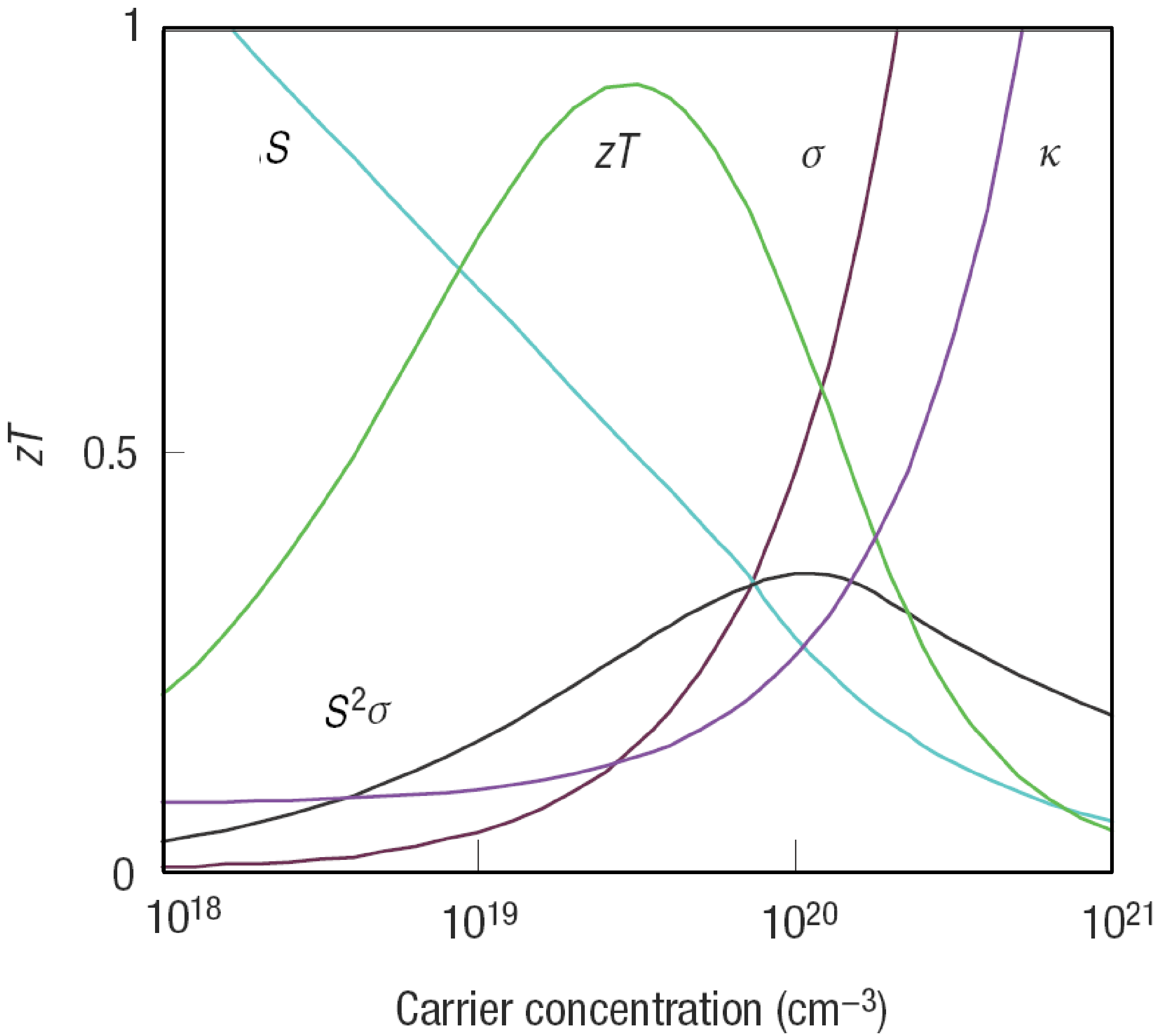
Thermoelectric element



After H. H. Saber, M. S. El-Genk, T. Caillat.
Energy Conv. Manag. 48 (2007) 555

Why materials science
is
important
for
thermoelectrics?

Thermoelectric figure-of-merit



n

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

$$S \sim m^*\frac{1}{n^{2/3}}T$$

$$\sigma = \frac{\tau \cdot e}{m^*}n$$

$$\kappa = \kappa_e + \kappa_l$$

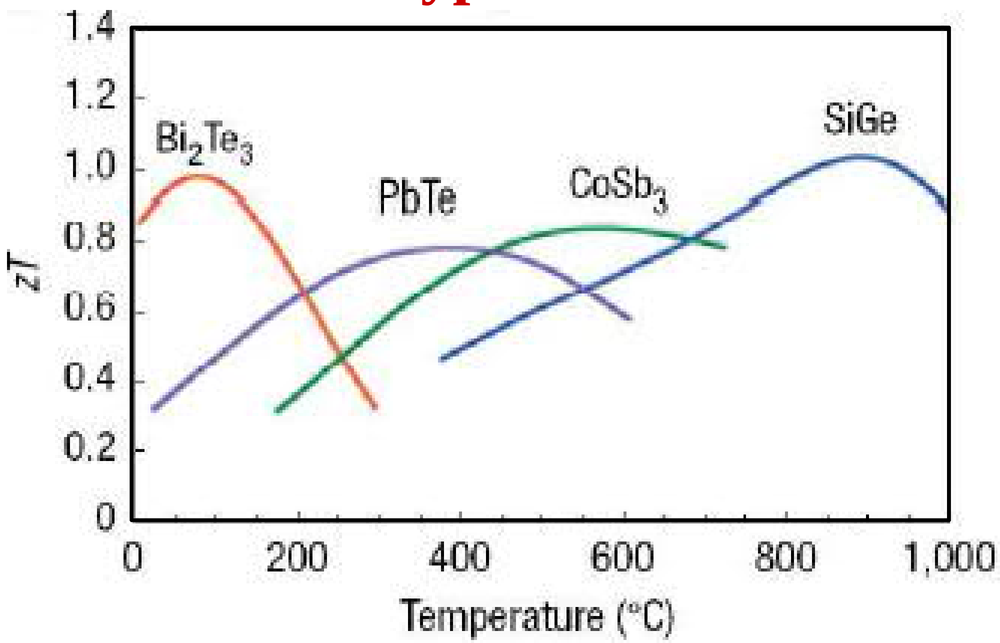
$$\kappa_e = L_0\sigma T$$

$$\kappa_l = \frac{1}{3}v_l\tau_l c_l$$

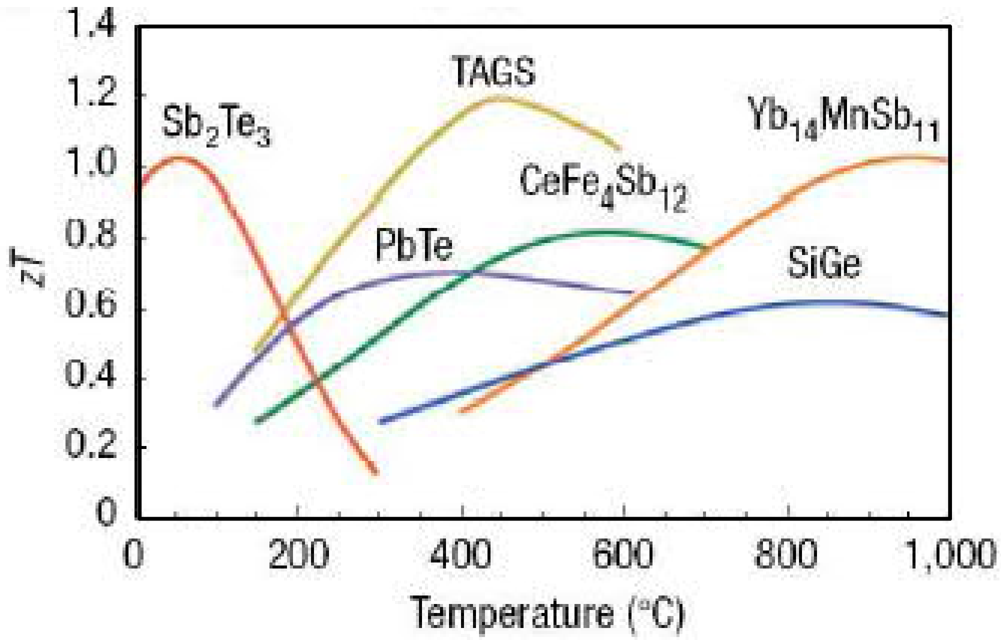
A. F. Ioffe, Semiconductor Thermoelements, 1960
G. Snyder and E. Toberer, Nature Mater. 7, 105 (2008)
S. Paschen, C. Godart, Yu. G. In: Complex Metallic Alloys: Fundamentals and Applications, WILEY-VCH (2011) 365

Temperature dependence of the thermoelectric efficiency

n-type materials

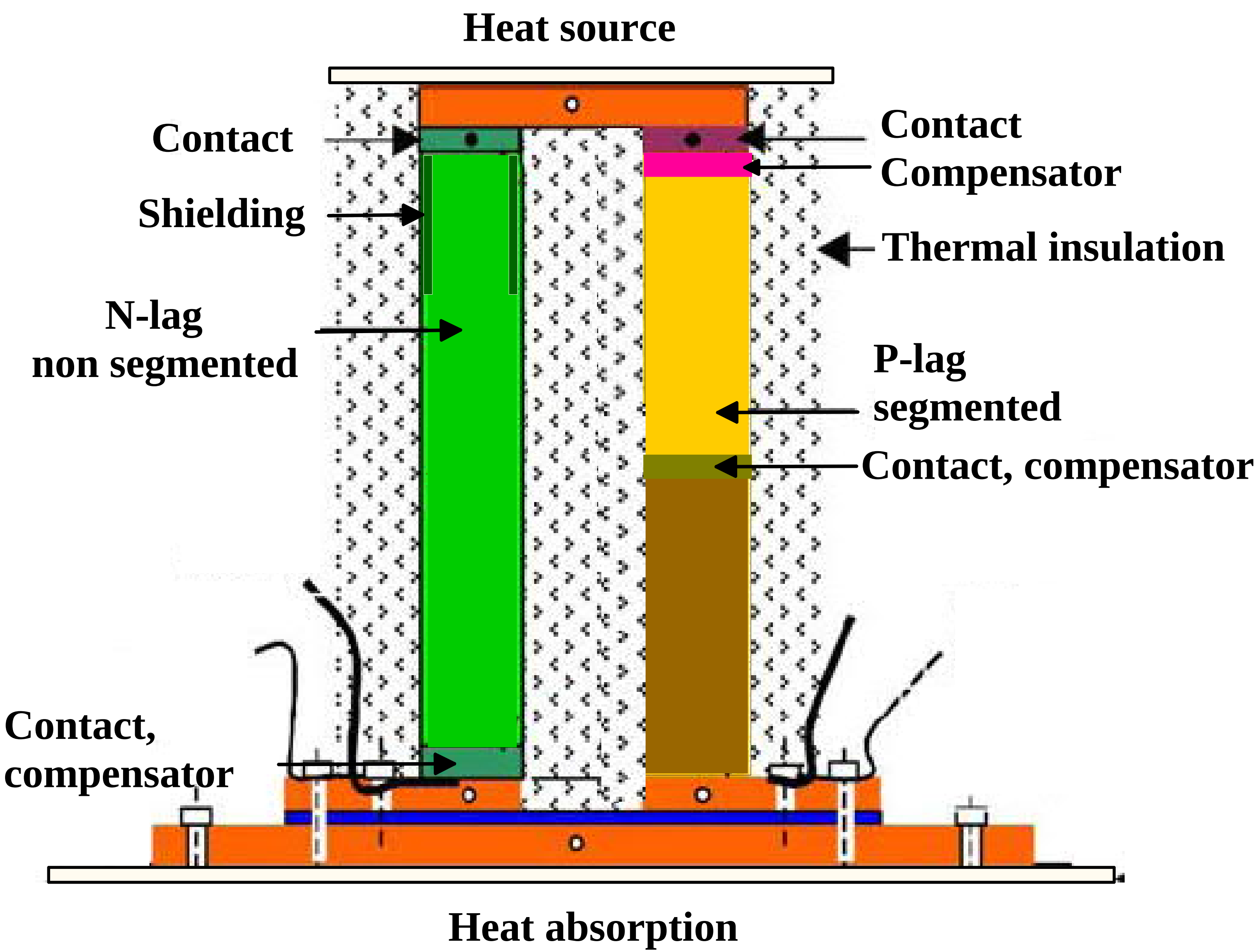


p-type materials



C. Godart, A. Goncalves, E. B. Lopes, B. Villeroy. MRS Symp. Proc. 1166 (2009) 183

Materials interaction in thermoelectric module



After H. H. Saber, M. S. El-Genk, T. Caillat.
Energy Conv. Manag. 48 (2007) 555

Good thermoelectric material should be ...

a semiconductor with

- high charge carrier mobility:
  high θ_D,
  low ionicity (high covalency), not for C-Si-Ge-Sn row
  heavy atoms forming more diffuse covalent bonds
  low effective mass (not decisive)
- low thermal conductivity:
  low mean free path
  (influenced by fluctuations of thermal motion and defects
  i.e. deviations from the translational symmetry)
  isoelectronic (isomorph) substitutions

and

- suitable for self- or substitutional doping, approx. $>10^{19}$ cm^{-3}

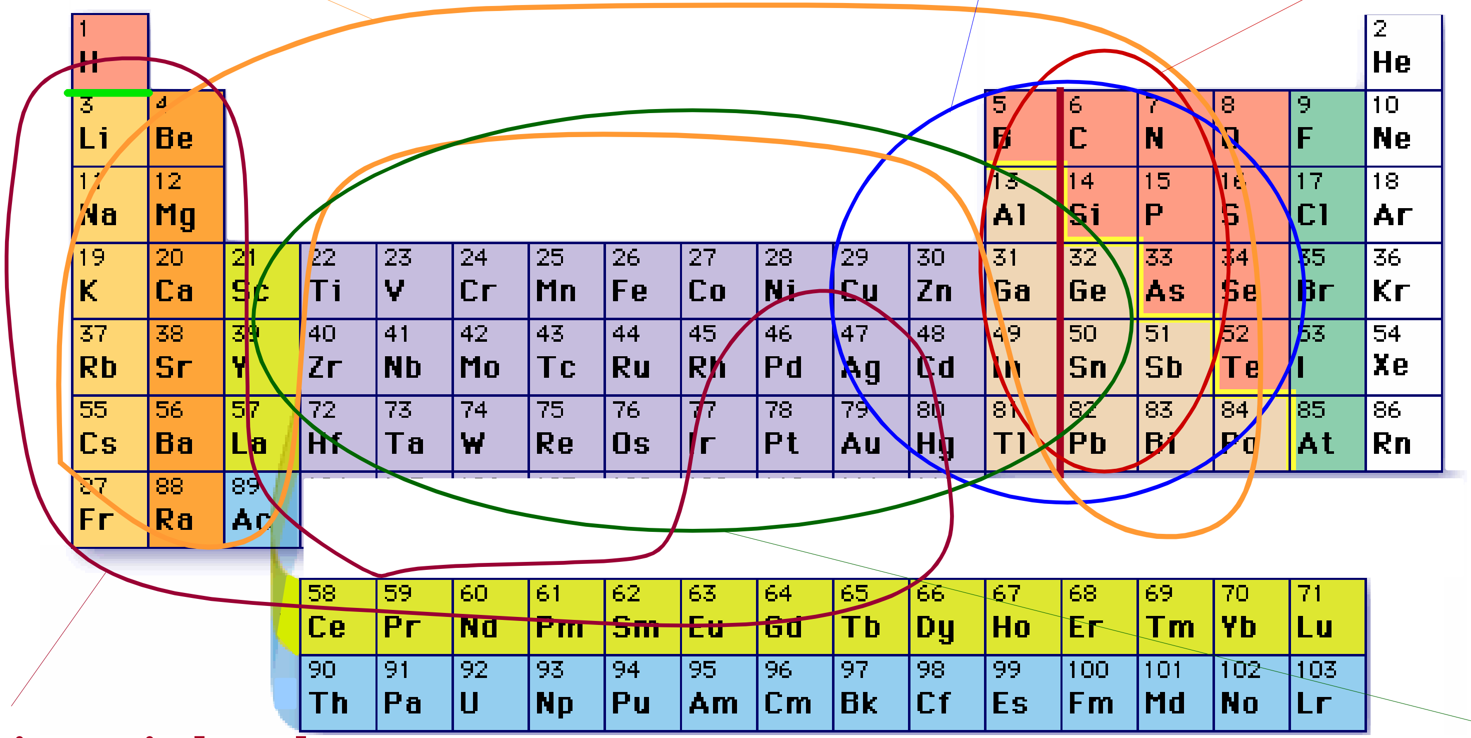
A. F. Ioffe. Semiconducting thermoelements. (1960) 84ff.

Semiconducting arrangements ...

Strong charge transfer cation-anion,
2- and multiatomic bonds in the anion,
moderate polarity
$Yb_{14}MnSb_{11}$, skutterudites

2-atomic bonds,
moderate polarity
Bi_2Te_3, Sb_2Te_3, PbTe

2-atomic bonds,
non-polar and close
Si(Ge)



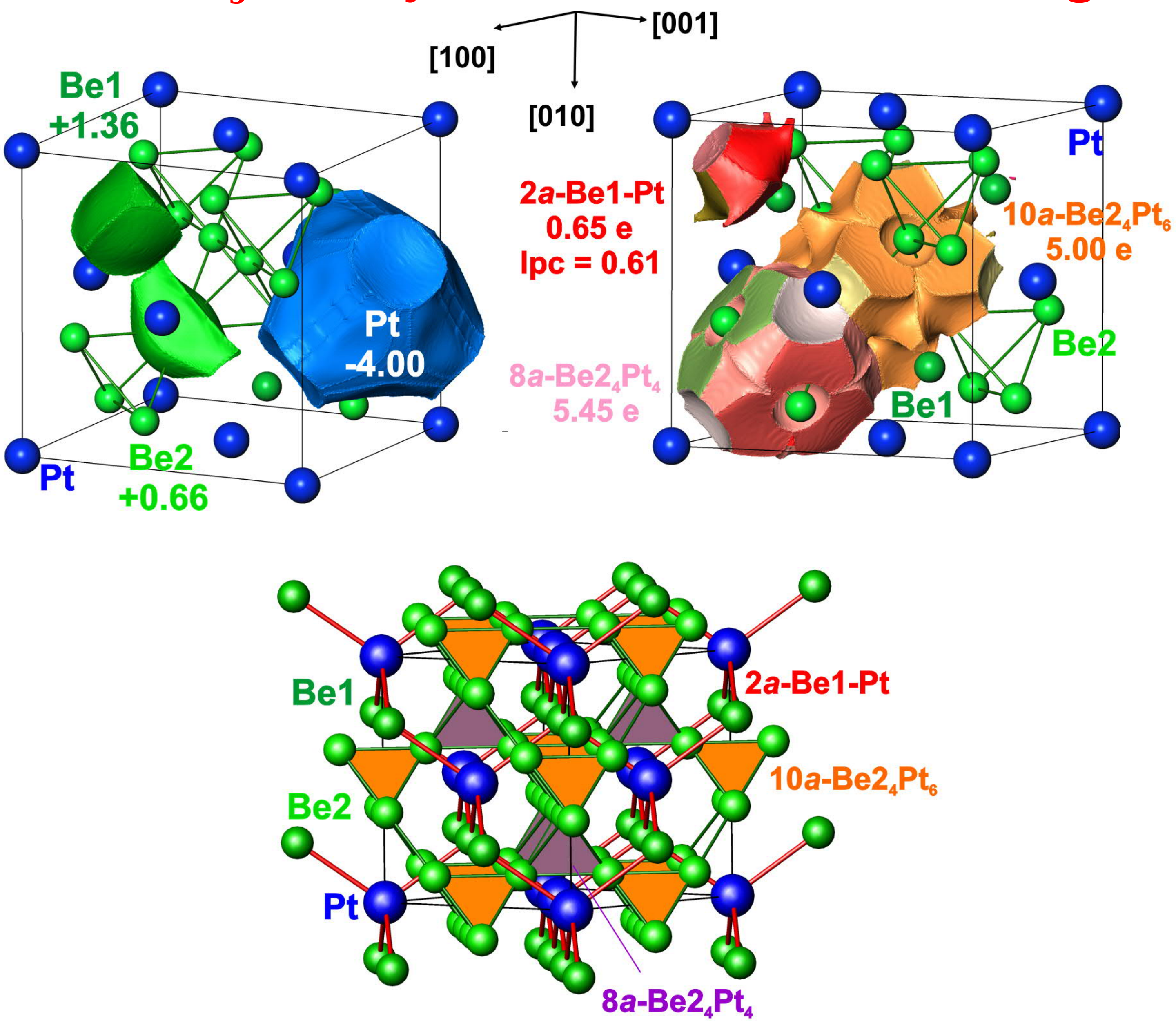
2- and multiatomic bonds,
strong charge transfer
?

2- and multiatomic bonds,
moderate polarity
CdSb

Yu. G. (2021) unpublished

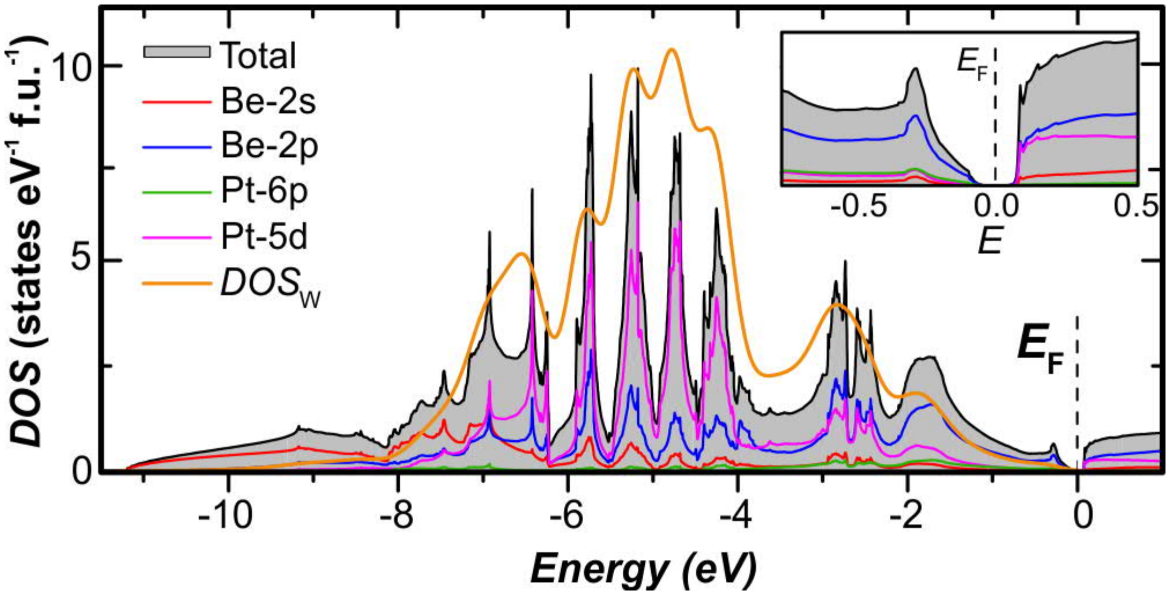
A. Amon, A. Ormeci, M. Bobnar, L. Akselrud, M. Avdeev, R. Gumeniuk, U. Burkhardt, Y. Prots, Ch. Hennig, A. Leithe-Jasper, Yu. G.. Acc. Chem. Res. 51 (2018) 214

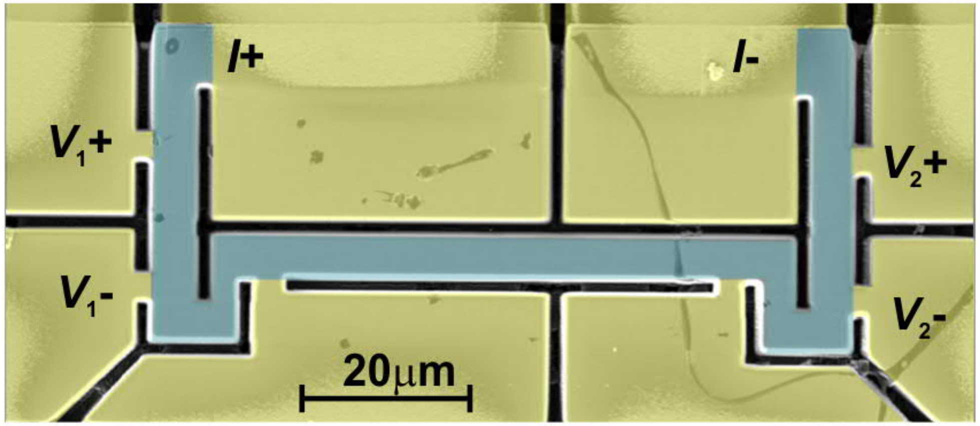
Be_5Pt: Crystal structure and bonding

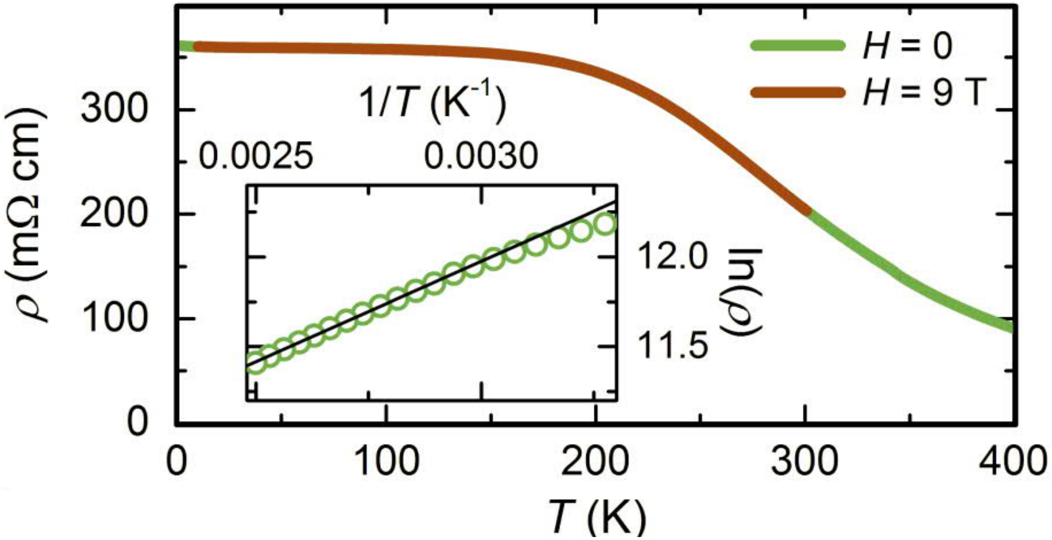


A. Amon, E. Svanidze, A. Ormeci, M. König, D. Kasinathan, D. Takegami, Y. Prots, Y.-F. Liao, K.-D. Tsuei, L. H. Tjeng, A. Leithe-Jasper, Yu.G. Angew. Chem. Int. Ed. 58 (2019) 15928

Be_5Pt: Semiconducting state







A. Amon, E. Svanidze, A. Ormeci, M. König, D. Kasinathan, D. Takegami, Y. Prots, Y.-F. Liao, K.-D. Tsuei, L. H. Tjeng, A. Leithe-Jasper, Yu.G. Angew. Chem. Int. Ed. 58 (2019) 15928

Conclusions

- Chemical bonding is a basis for electron and phonon engineering as well as for the preparation of new thermoelectric materials

- Spatial distribution of the regions with different types of chemical bonding - inhomogeneity and anisotropy - influences thermal transport more than other chemical or crystallographic features

Courtesy NASA/JPL-Caltech/Space Science Institute