Solid State Energy Harvesting and Power Conversion in Gas Turbine Engines

NASA Aeronautics Research Institute

$$J = AT^2 e^{-\left(\frac{E_w}{kT}\right)}$$

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

Jon Goldsby, Ph.D., MBA Engineer NASA Glenn Research Center

NASA

United Technologies
Research Center

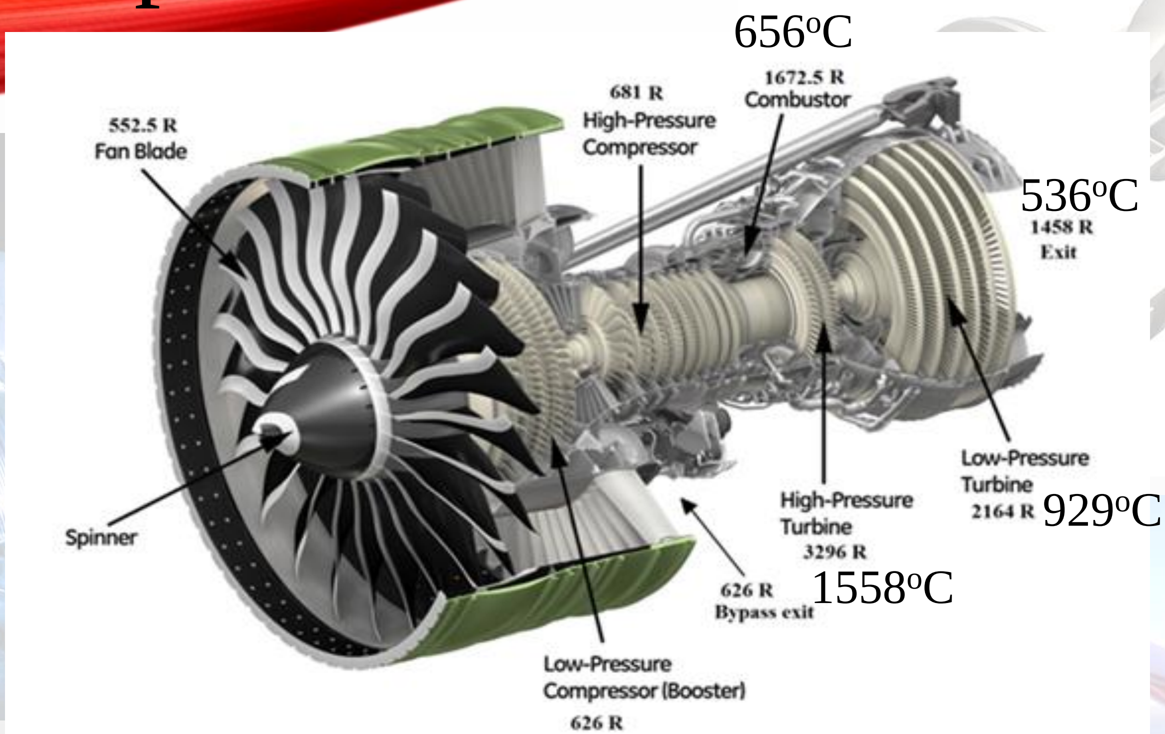
Air Force Research Laboratory

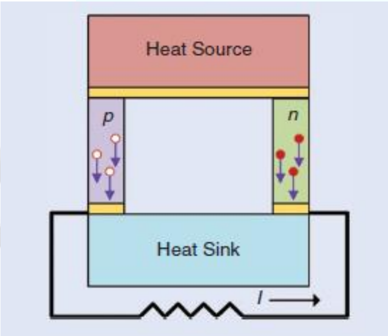
Case Western Reserve
Est. 1826 University
think beyond the possible

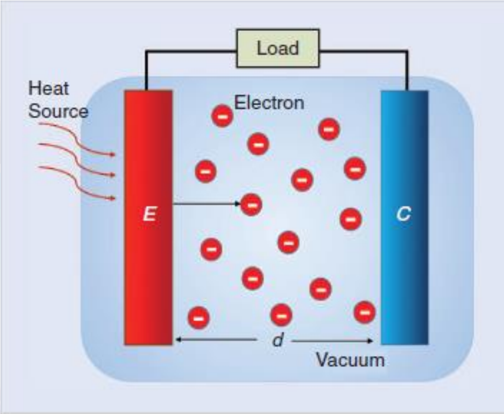
Air Force Office of Scientific Research
United States Air Force

Purdue
University

Concept Overview

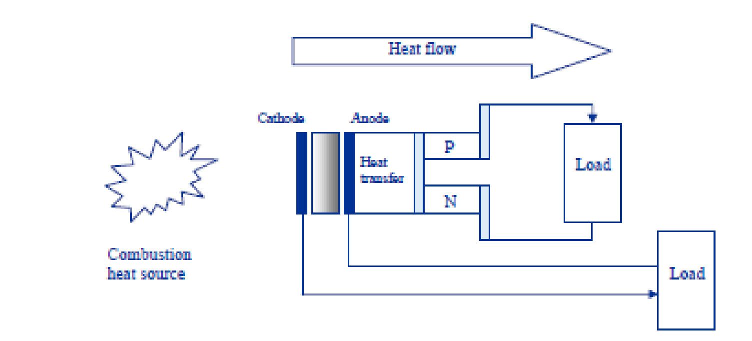


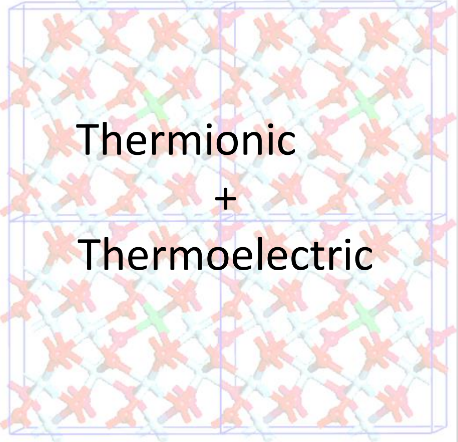




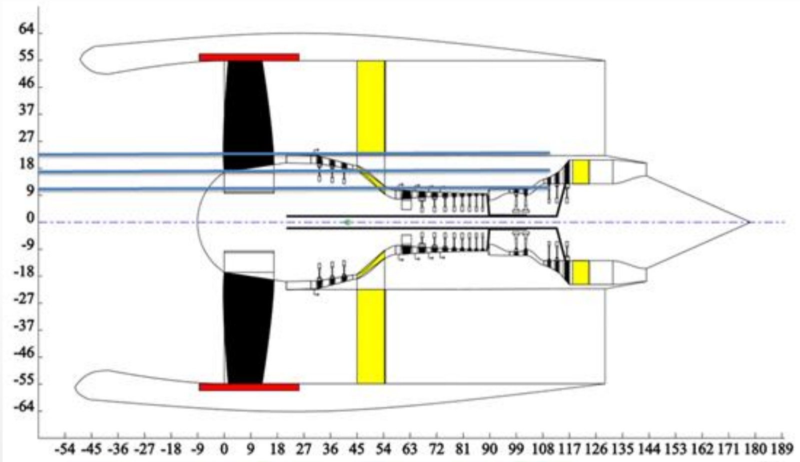
$$AT^2 e^{-\left(\frac{E_W}{kT}\right)}$$

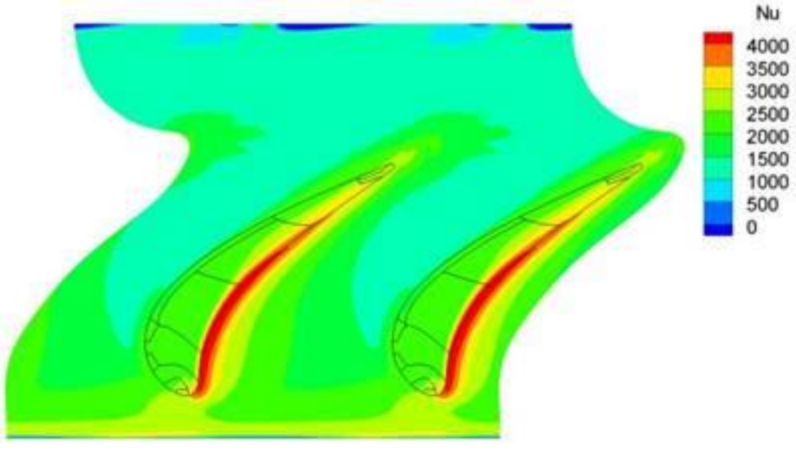
- Solid state energy harvesting using waste heat available in gas turbine engine offers potential for power generation to meet growing power needs of aircraft
- Thermoelectric material advances offer new opportunities
- Weight-optimized integrated turbine engine structure incorporating energy conversion devices

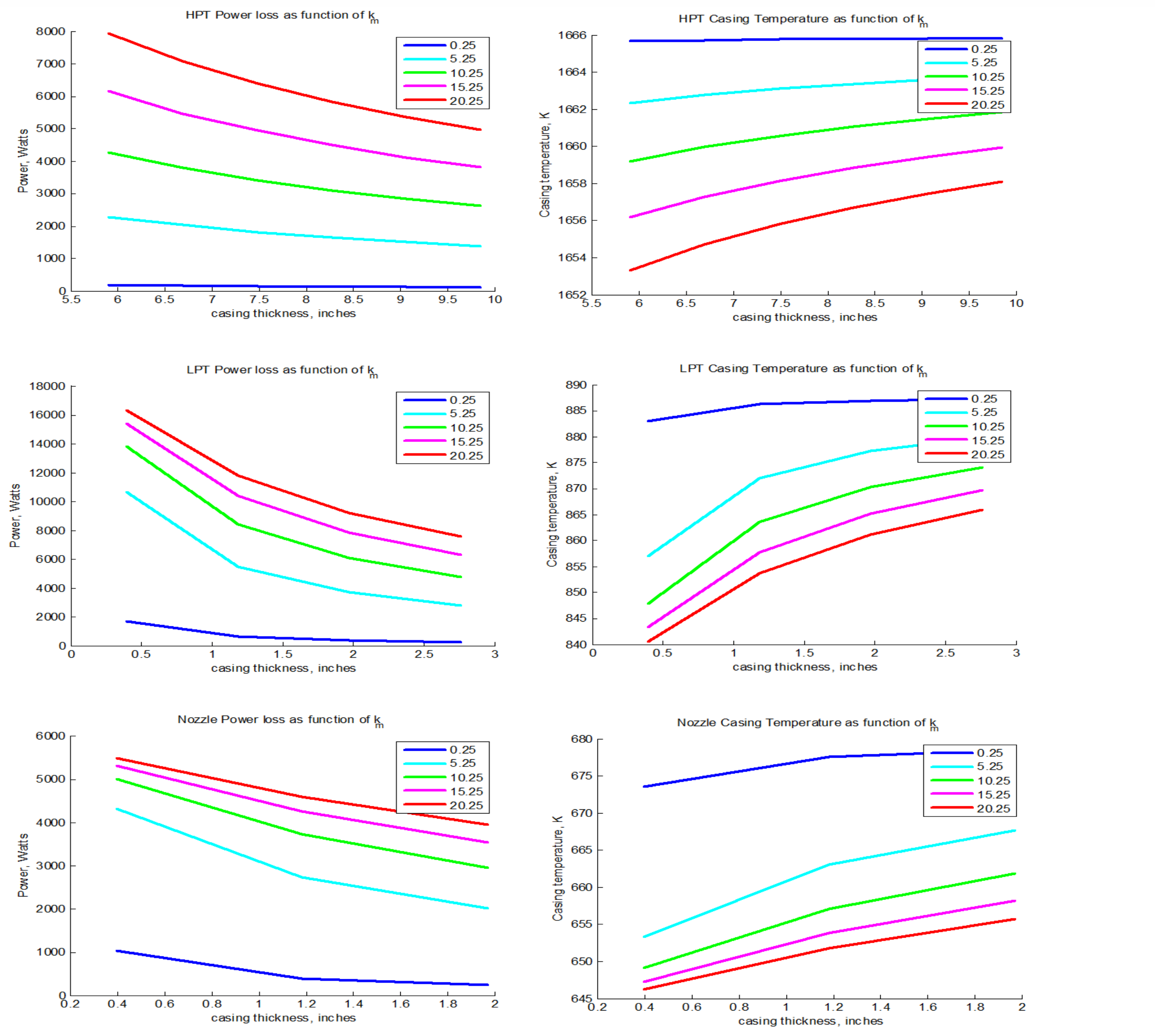




Calculated power available in various Parts of the gas turbine engine

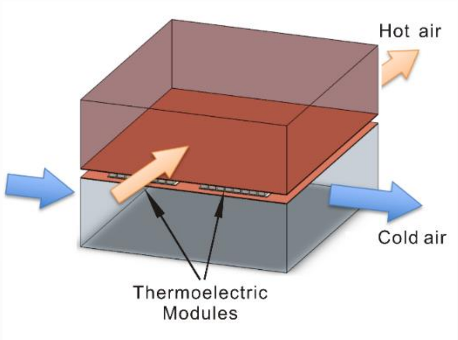


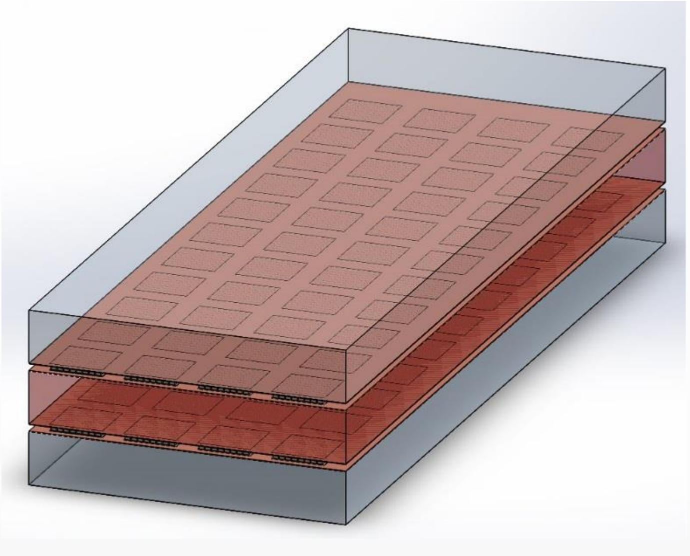




Utilization Concept: Heat Exchanger

Type of heat exchanger: Counter flow





- **One hot air channel and two cold air channels.**
- **Hot air channel is between cold air channels.**

Parametric Optimization of Thermoelectric Generators for Waste Heat Recovery *Shouyuan Huang, Xianfan Xu*
Journal of Electronic Materials 45(10) · June 2016

Skutterudite based modules from Marlow Industries

Results – 1, cold air T = -35ºC

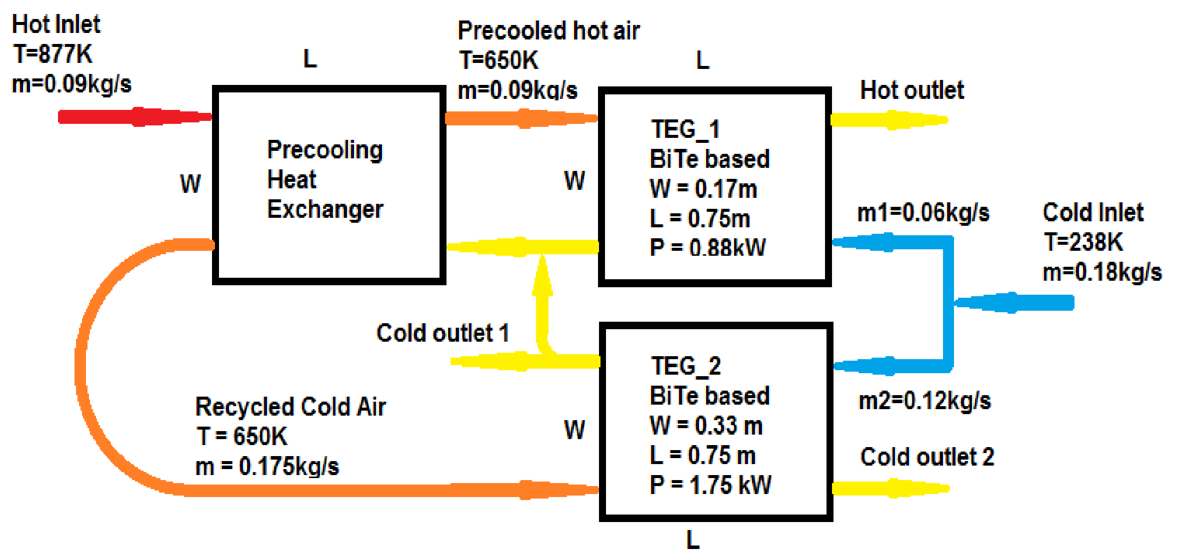
Integral treatment 1, Counter flow, $\dot{m}_h = 0.09kg/s$; $T_{hot,in} = 604$°C;

Cold inlet: $T_{cold} = -35$°C, $\dot{m}_{cold,total} = 0.18kg/s$

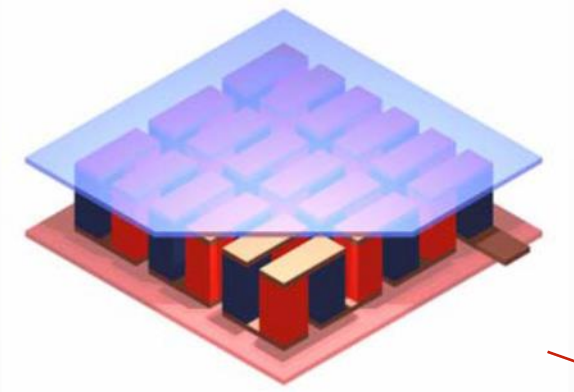
TEG hot inlet: $T_{hot,inlet,TEG} = 377$°C

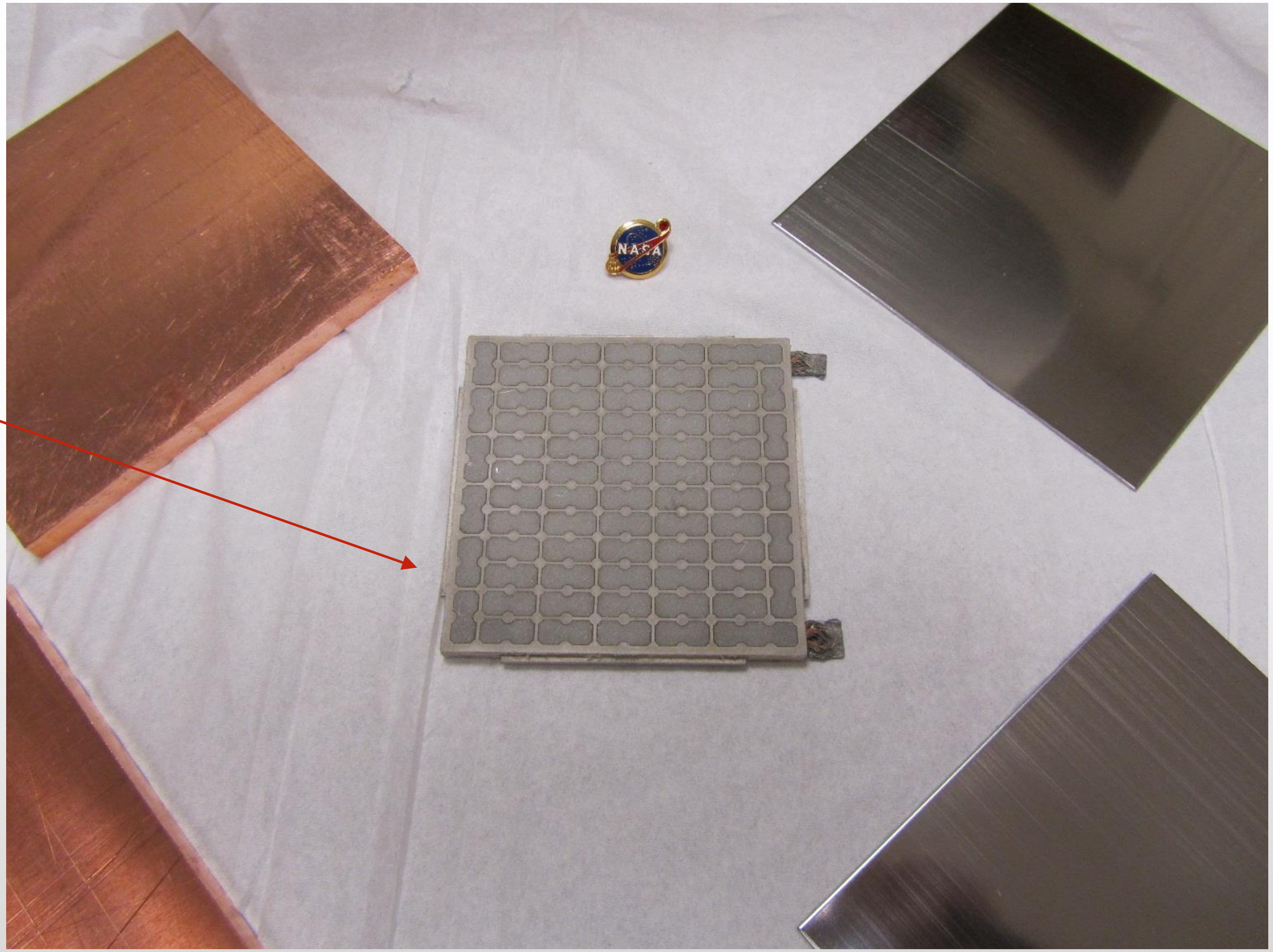
$m_{Bi_2Te_3}$(kg)	$\dot{m}_{recycle}$ (kg/s)	$T_{cold,out,TEG}$ (C)	P_{total} (kW)	P_1 (kW)	P_2 (kW)	Q_{total} (kW)
1.73	0.175	256	**2.64**	0.88	1.75	40.45

Design of TEG	
$A_{precool}$	0.016 m^2
W_{TEG_1}	0.17 m
L_{TEG_1}	0.75 m
W_{TEG_2}	0.33 m
L_{TEG_2}	0.75 m
h_{leg}	1.3 mm



Thermoelectric generator Module Bi_2Te_3

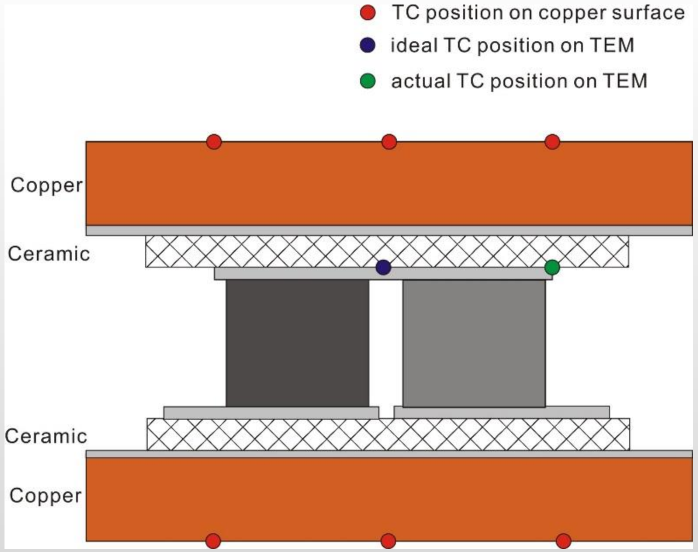




Test Setup

Measurements

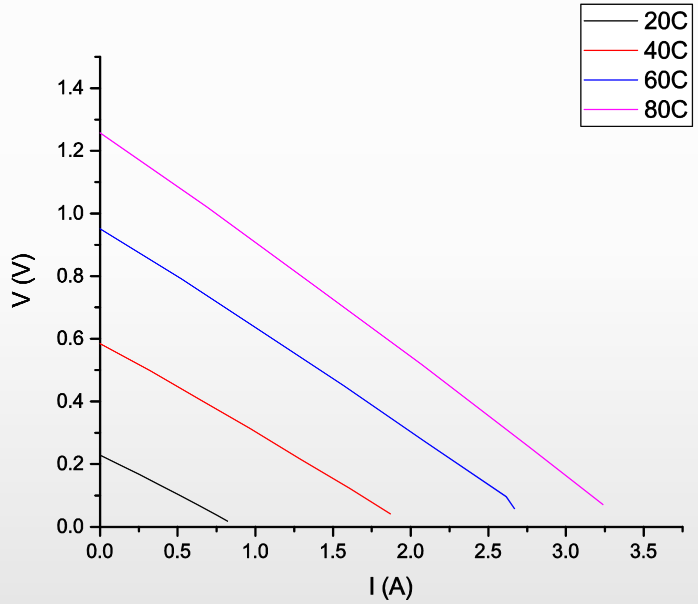
- Bi_2Te_3 module
- Module is kept in the package for electrical insulation and mechanical contact reasons.
- TCs mounted on copper surfaces (T_TEMH1-3, T_TEMC1-3), thus ΔT measured includes metal bulk and interface resistance of metal and ceramic.
- Unable to put TCs inside, at edge of TEM (T_TEMH4, T_TEMC4) instead to estimate thermal resistance between copper surfaces and TEM surfaces

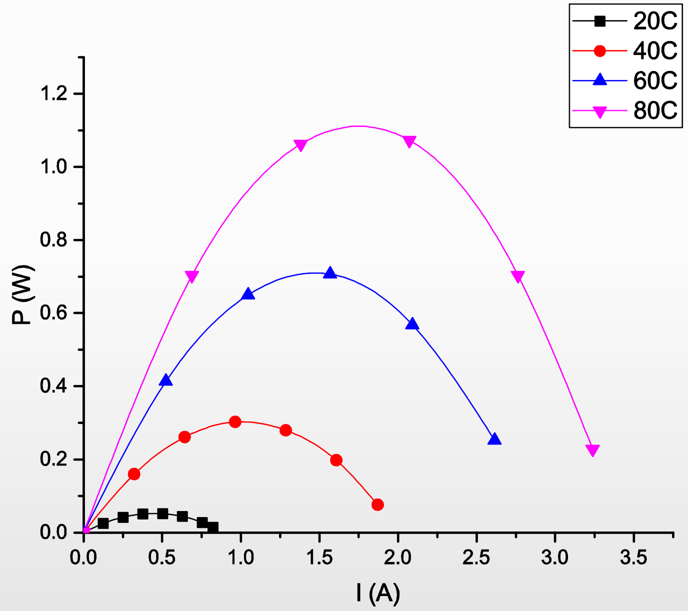


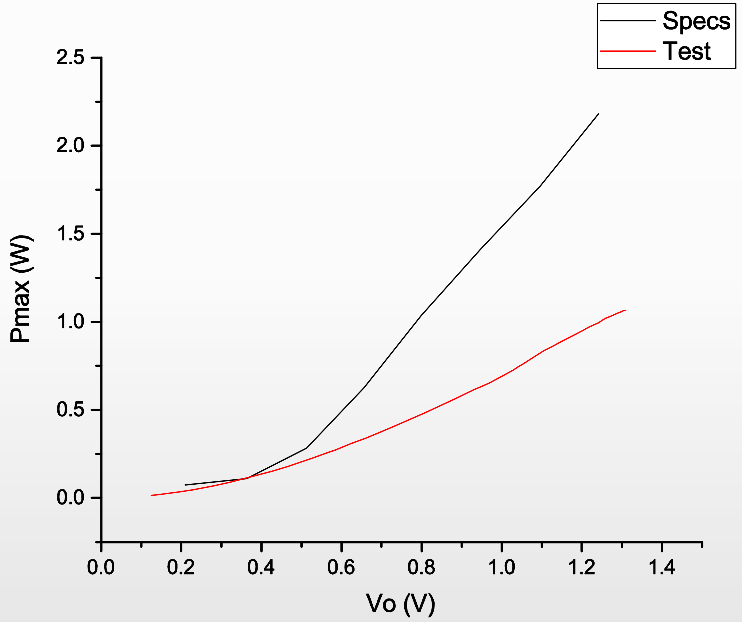
Test Results

Bi2Te3 module

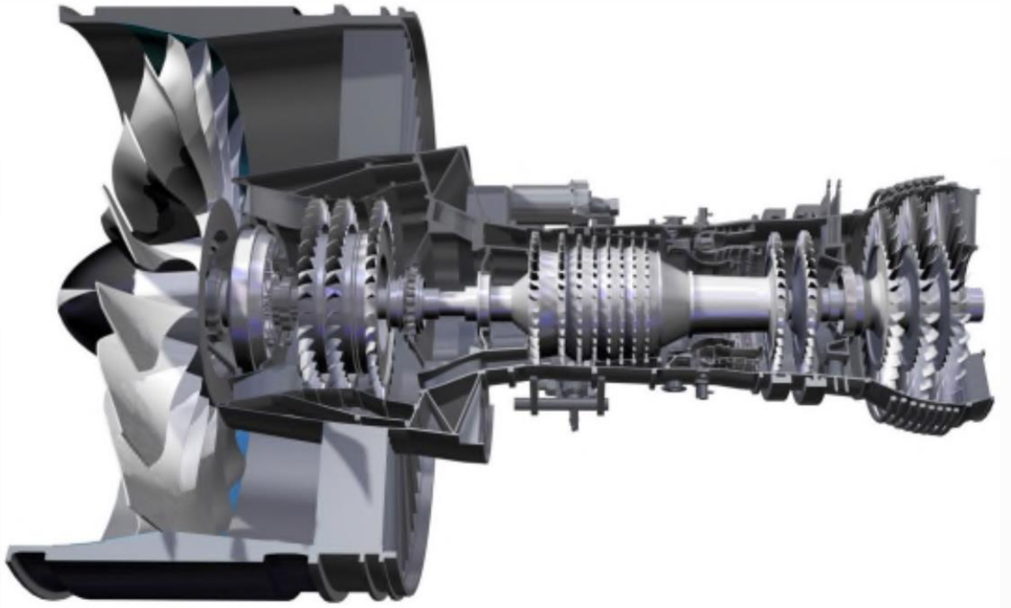
IV sweep were taken (left figure below) and the maximum power was obtained at each ΔT.







Pratt & Whitney PW1000G Geared Turbofan™



- **Heat Exchangers** - TEGs cause significant gains in weight and size due to thermal resistance
- **Surfaces**

- LPC – Miniscule opportunity (ΔT small)
- HPC – Small opportunity
- Diffuser – Single kW, but do not want to create hot spots or remove heat from cycle
- HPT and LPT – 10 kW contingent on avoidance of hot spots, TEG material robustness.
- **Distributed, small scale power generation for wireless sensors** on aircraft

appear promising. A TEG measuring approximately 1 in^2 generates 50 mW to power sensing and transmission circuits.

Characteristics for a desirable thermoelectric material

- Seebeck Coefficient ~ 100uV/K
- Electrical Resistivity 10^{-2} Ohm*cm
- Thermal Conductivity ~ 10 W/m*K
- Electronic Band Gap -must be greater than zero
- High Temperature Capability

Computational Methods

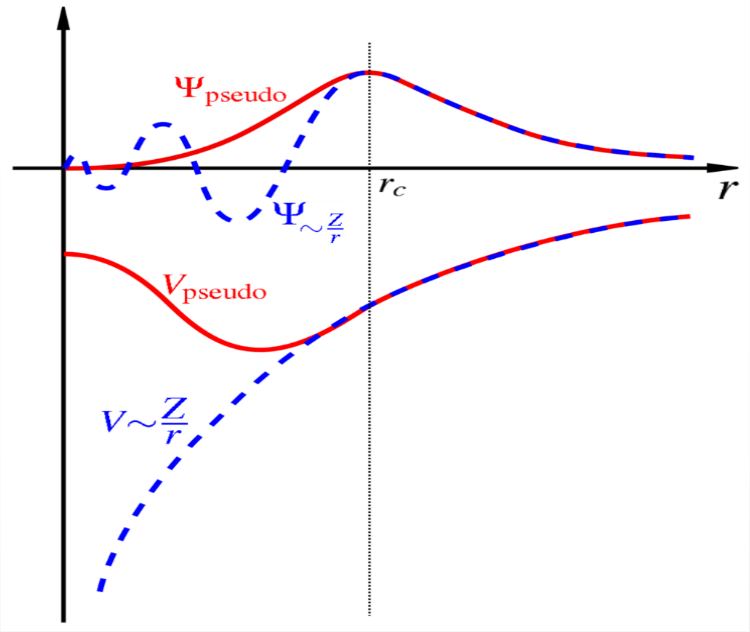
The Schrödinger Equation

$$\left[\underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)}_{\text{Hamiltonian operator}}\right]\underbrace{\psi(x)}_{\text{Wave function}} = \underbrace{E}_{\text{Energy}}\psi(x)$$

BoltzTraP. A code for calculating band-structure dependent quantities ☆

Georg K.H. Madsen [a,*], David J. Singh [b]

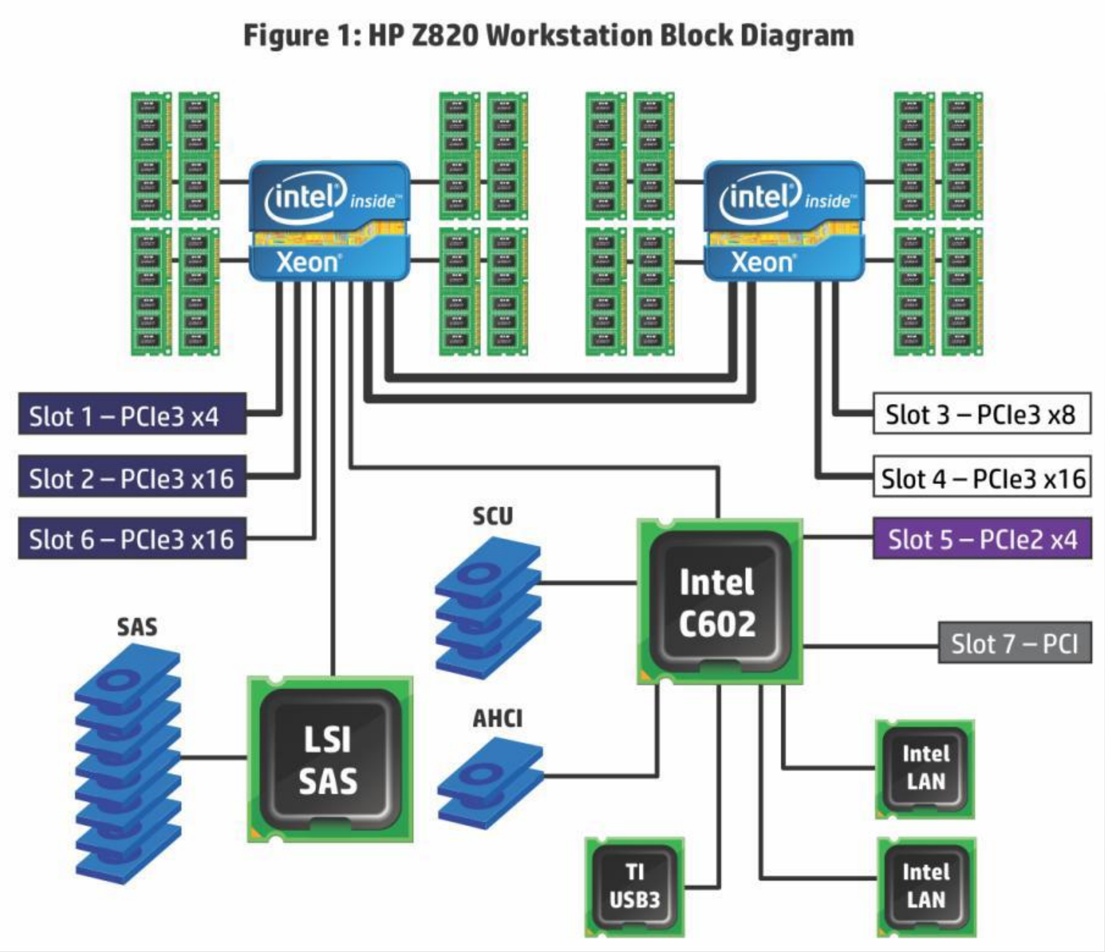
Computer Physics Communications 175 (2006) 67–71



Vienna Ab-initio Simulation Package

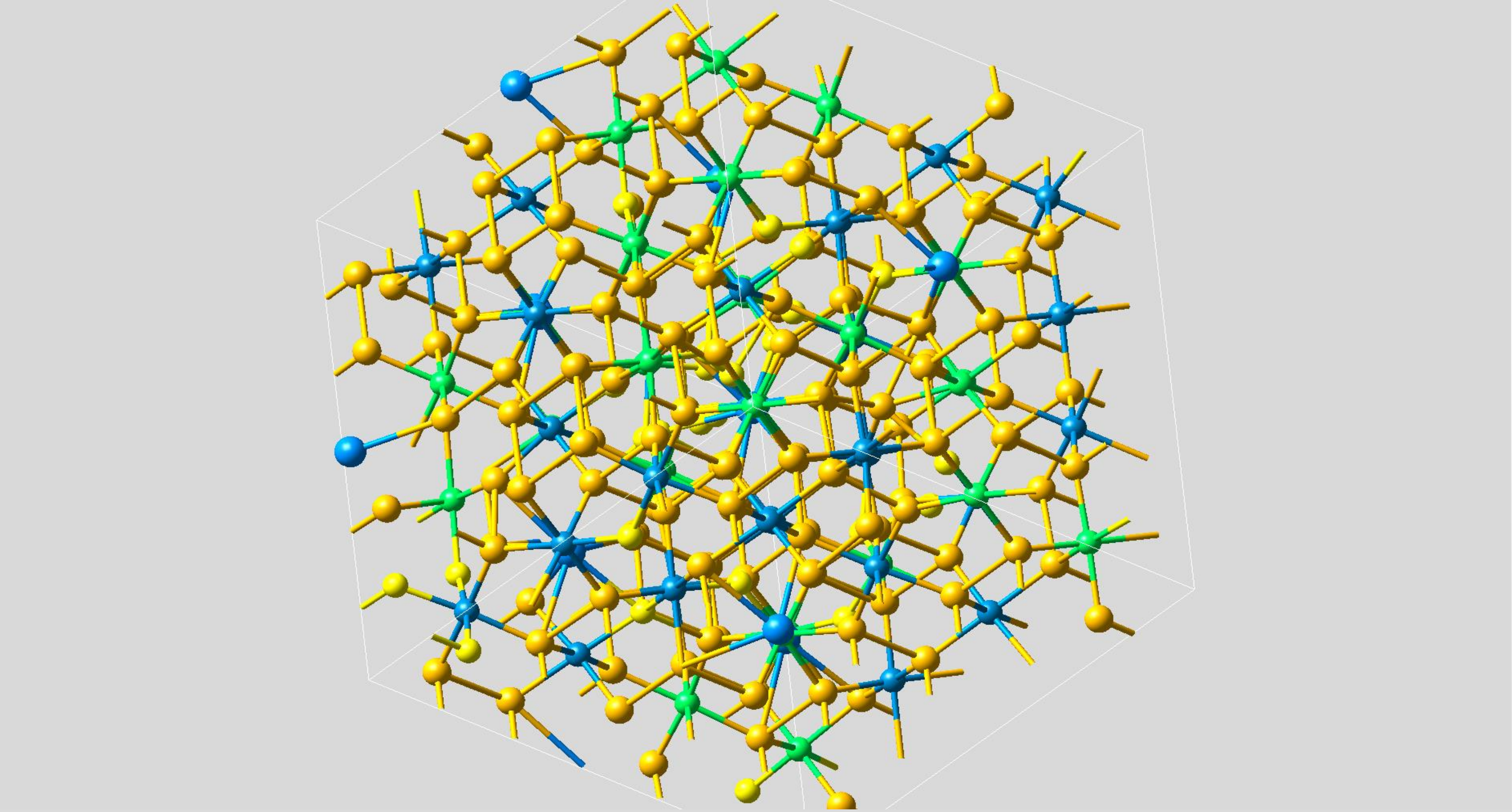
The Vienna Ab-initio Simulation Package, better known as **VASP**, is a package for performing ab initio quantum mechanical molecular dynamics using either Vanderbilt pseudopotentials, or the projector augmented wave method, and a plane wave basis set

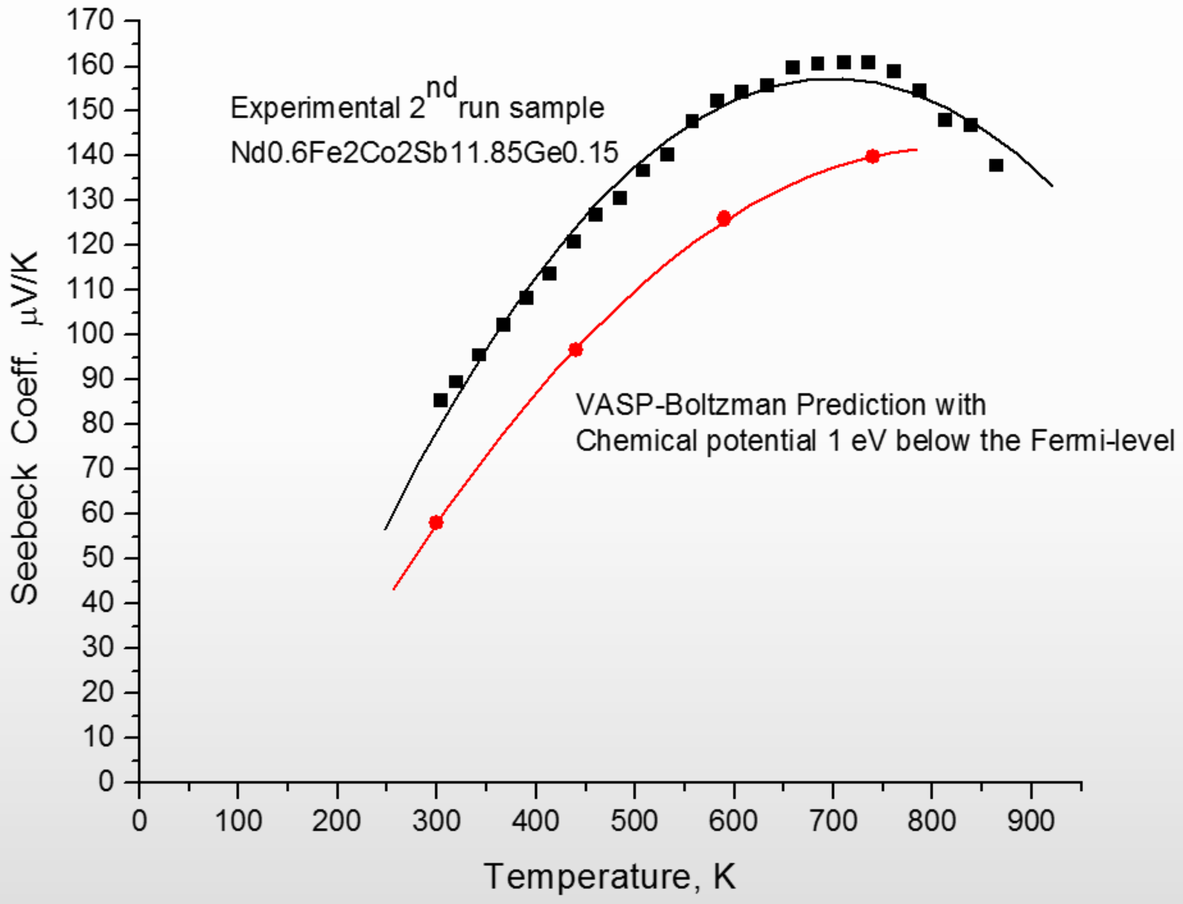
Computing Platform:
Hewlett-Packard Z840 Workstation
Dual 18-core intel Xeon processors
Widows 10 pro 64-bit
128 GB ram



HEWLETT PACKARD HP Z820 WORKSTATION 2 INTEL XENON PROCESSORS ALLOWING 32 CORES FOR CALCULATION WITH 192 GB OF RANDOM ACCESS MEMORY

Complex Skutterudites Thermoelectric (Mackey, Dynys)
Nd0.6Fe2Co2Sb11.85Ge0.15

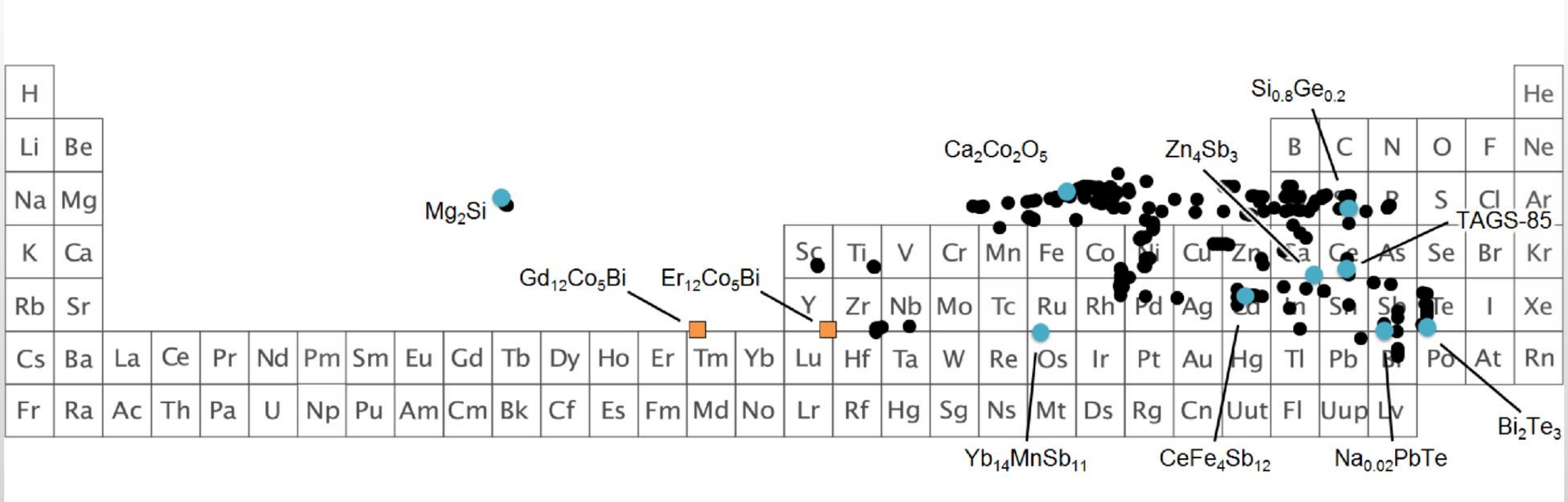



Experimental 2nd run sample
Nd0.6Fe2Co2Sb11.85Ge0.15
VASP-Boltzman Prediction with
Chemical potential 1 eV below the Fermi-level
Seebeck Coeff. μV/K
Temperature, K
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
0
100
200
300
400
500
600
700
800
900

A Recommendation Engine for Suggesting Unexpected Thermoelectric Chemistries

Michael W. Gaultois, Anton O. Oliynyk, Arthur Mar, Taylor D. Sparks, Gregory J. Mulholland, Bryce Meredig

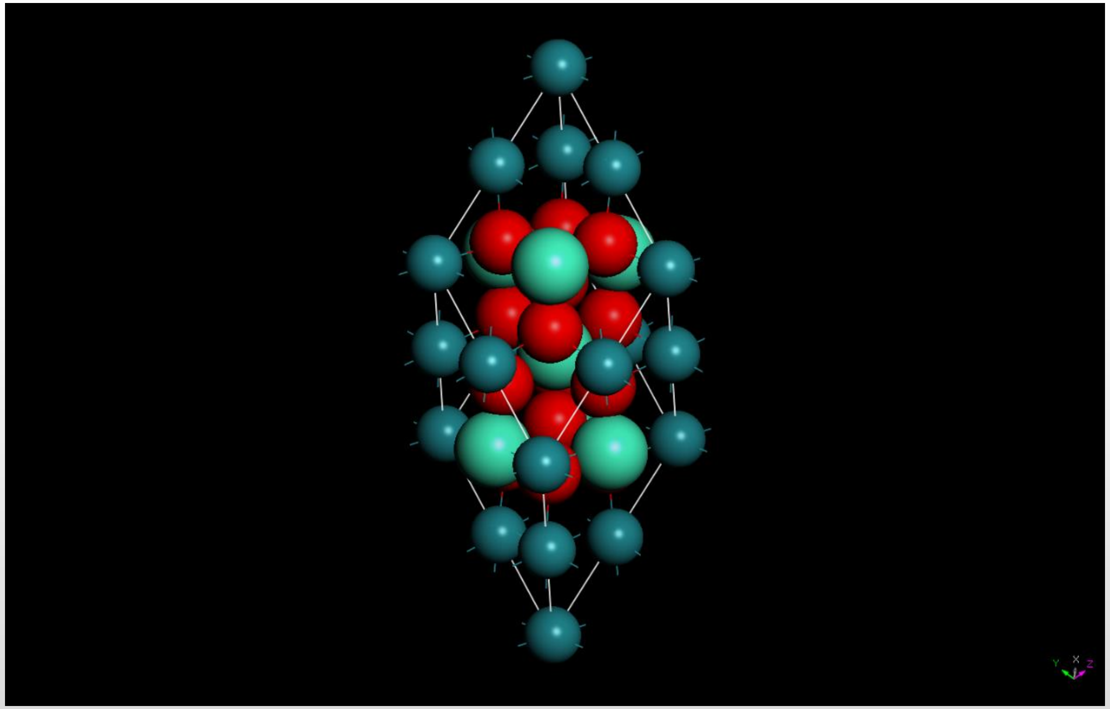
(27 Feb 2015)

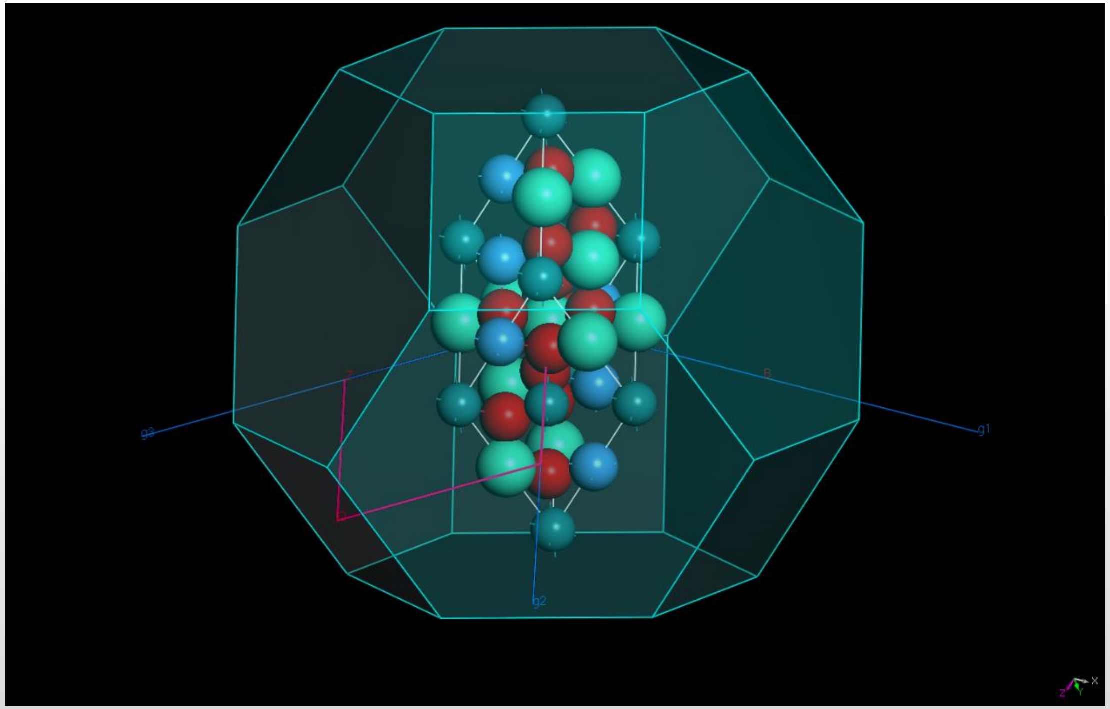


Complex Oxide – based Pyrochlores

mixed cation at B-site $A_2 (B^{3+}, B^{\sim 5+}) O_7$

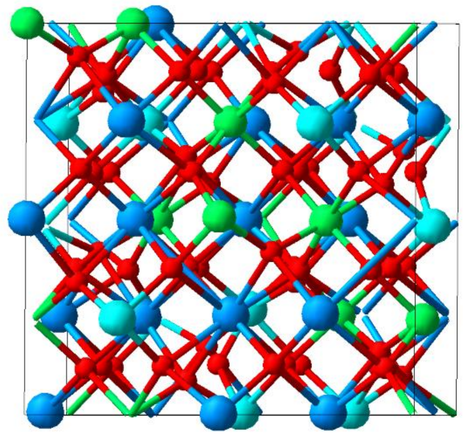
Gd_2RuTaO_7





Provisional utility patent application was filed NASA Docket No.: LEW 19688-1

Calculated Cell Parameters



Parameter	Original	change	Final	%
a	10.091900	0.158505	10.250405	1.6
b	10.091900	0.137867	10.229767	1.4
c	10.091900	0.156757	10.248657	1.6
alpha	90.000000	-0.361354	89.638646	-0.4
beta	90.000000	0.392175	90.392175	0.4
gamma	90.000000	0.047839	90.047839	0.1
Volume	1027.824144	46.795542	1074.619686	4.6

Density: 8.759 Mg/m^3

Elastic constant matrix (GPa):

	1	2	3	4	5	6
1	303.99	122.74	112.40	0.00	0.00	0.00
2	122.74	342.62	128.66	0.00	0.00	0.00
3	112.40	128.66	289.89	0.00	0.00	0.00
4	0.00	0.00	0.00	98.03	0.00	0.00
5	0.00	0.00	0.00	0.00	76.22	0.00
6	0.00	0.00	0.00	0.00	0.00	88.62

Modulus	Voigt	Reuss	Hill	
Bulk	184.90	183.56	184.23	GPa
Shear	90.75	89.78	90.27	
Young's	233.98	231.59	232.78	
Longitudinal			304.59	

Velocity of sound

Calculated from Hill moduli:

transverse waves: 3271 m/s

longitudinal waves: 6009 m/s

mean: 3649 m/s

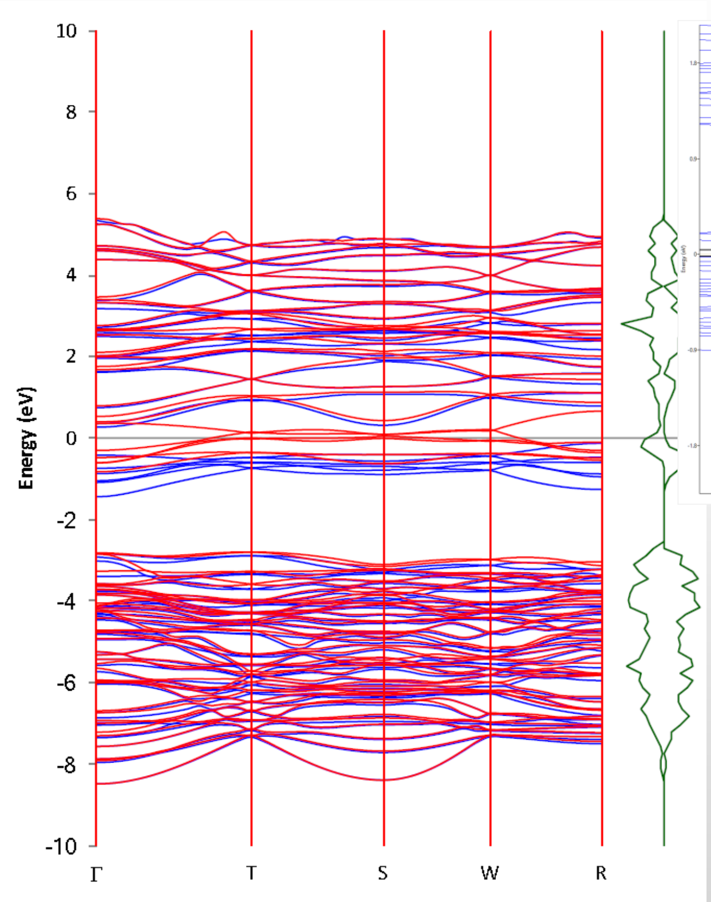
Debye temperature: 465.9 K

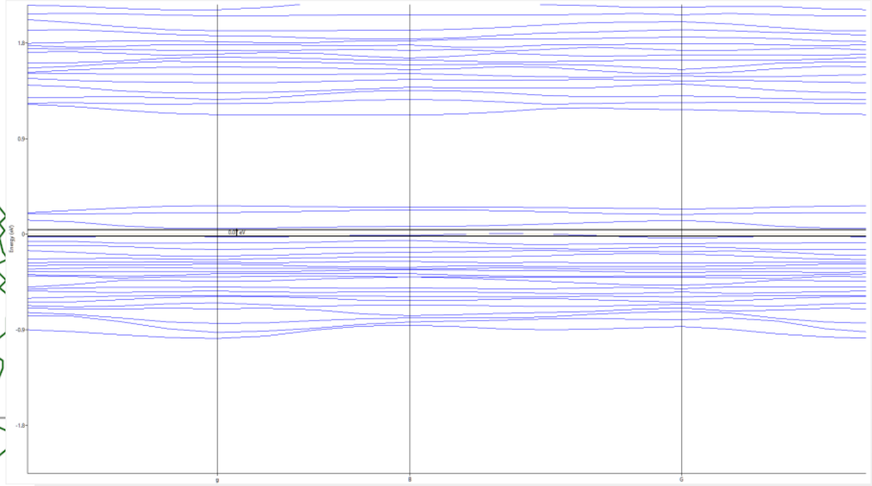
the thermal coefficient of linear expansion at 600K = 7.60×10^{-6}

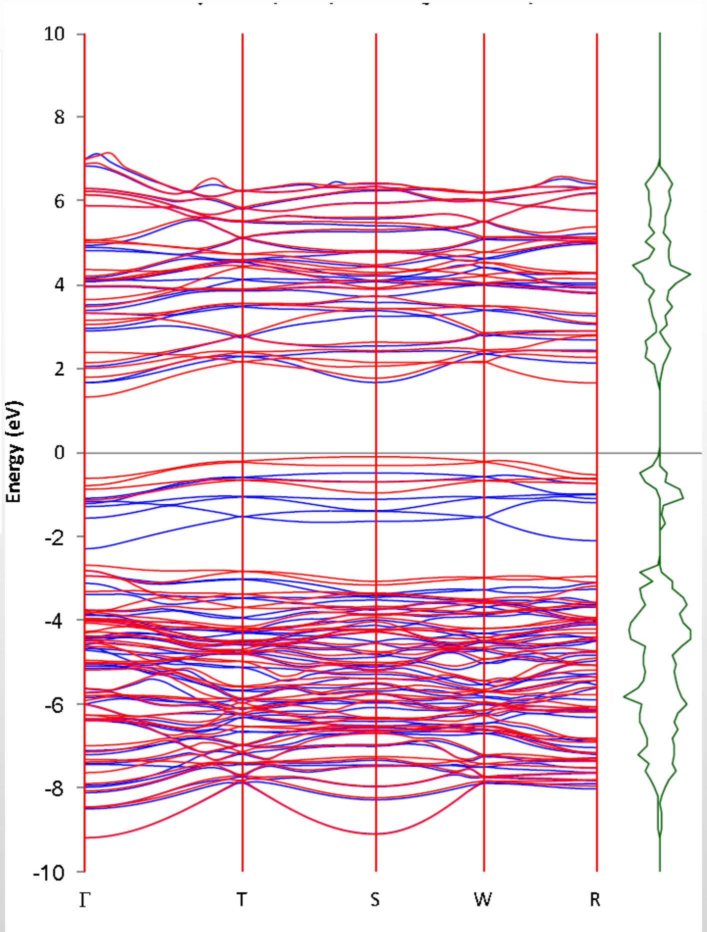
Calculated Electronic Band Structure

Perdew – Ernzerhof – Burke (PBE)

Heyd –Scuseria -Ernzerhof (HSE06)

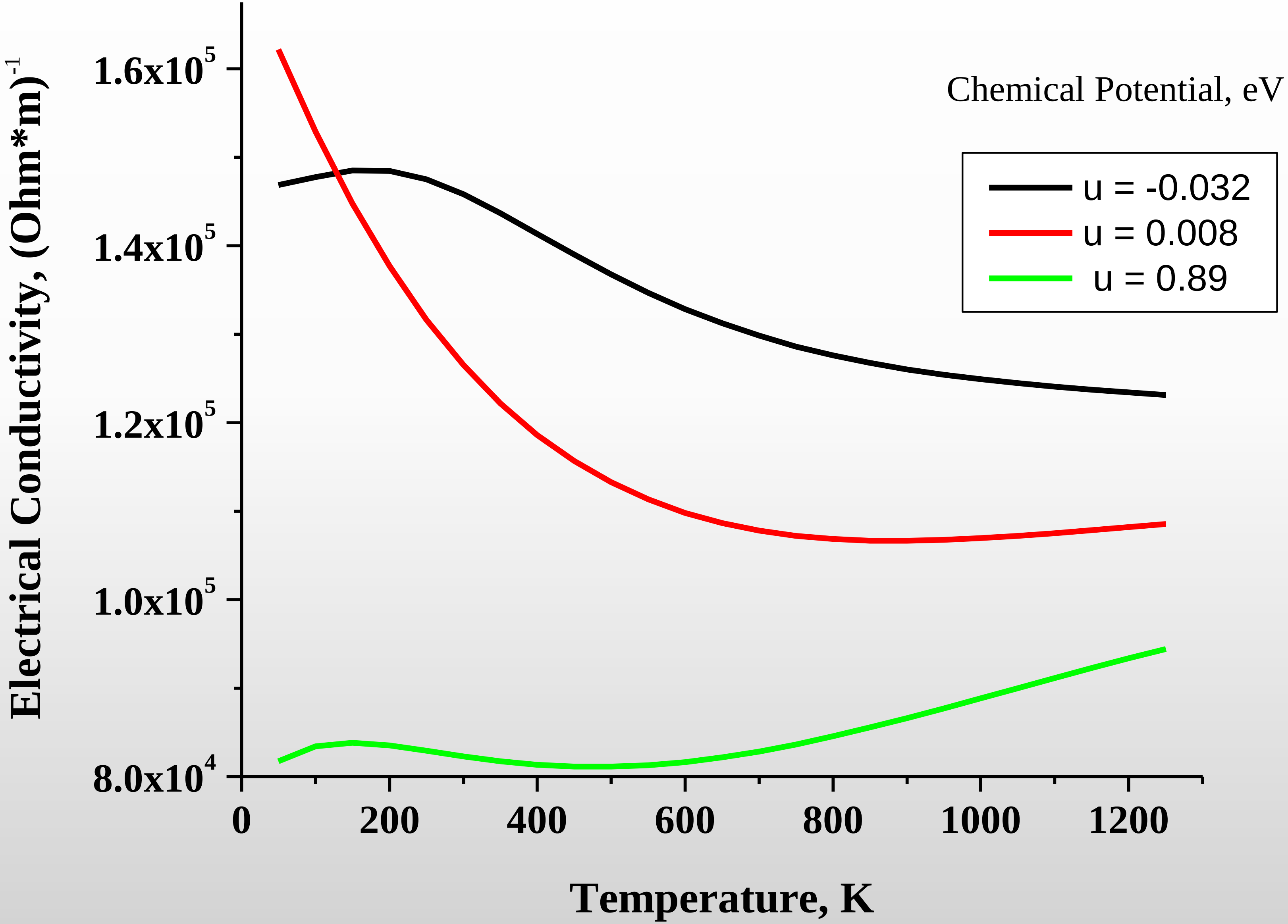




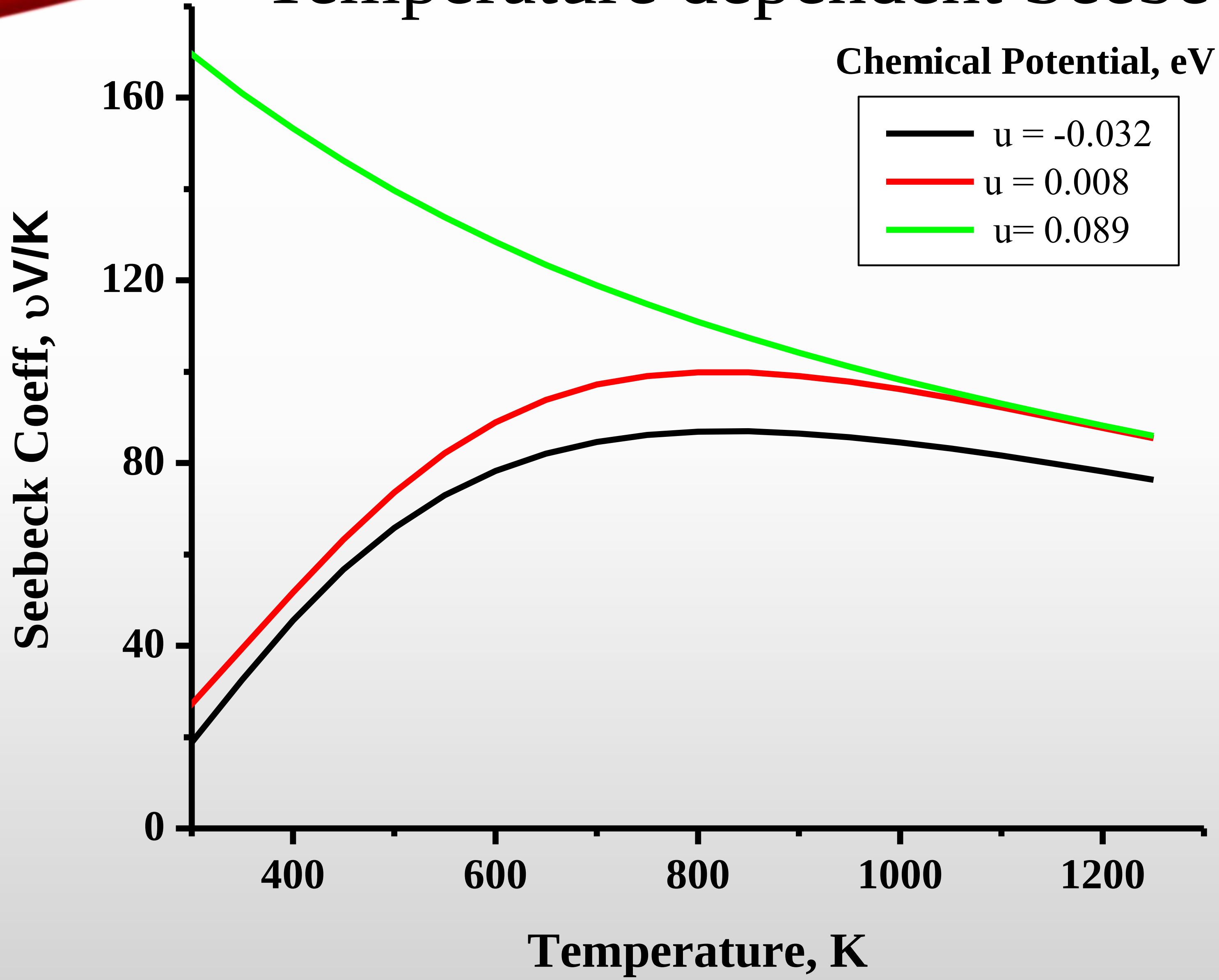


Cut off energy of 575 eV k-spacing 0.199/ A and 4x4x4 k mesh using DFT PBE the bandgap is 0.07 eV

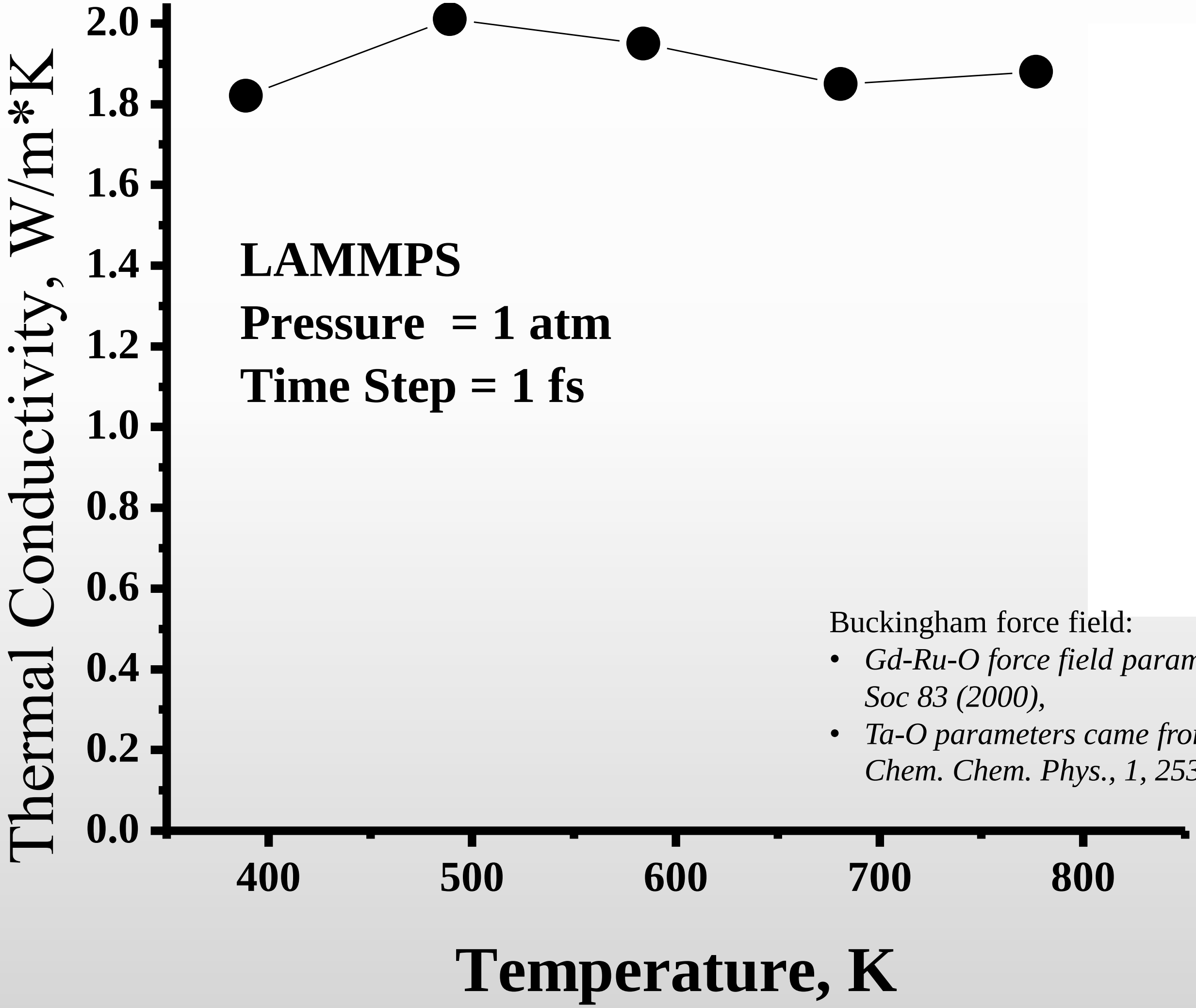
Electrical Conductivity

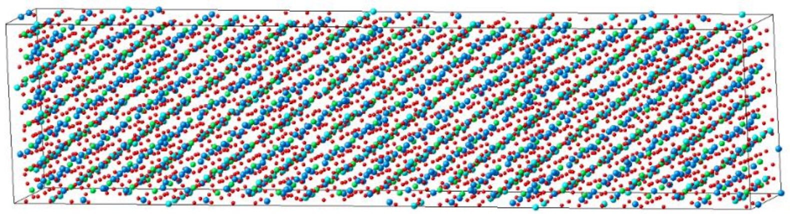


Temperature dependent Seebeck coefficient



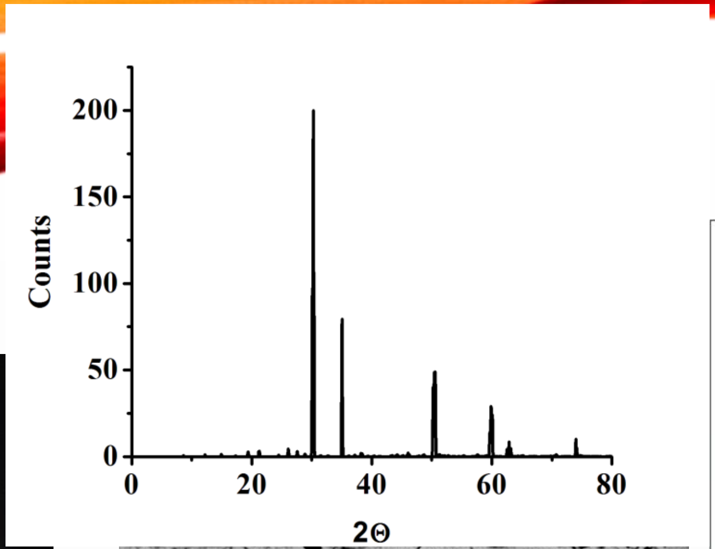
Molecular Dynamic Computational Results:
Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)

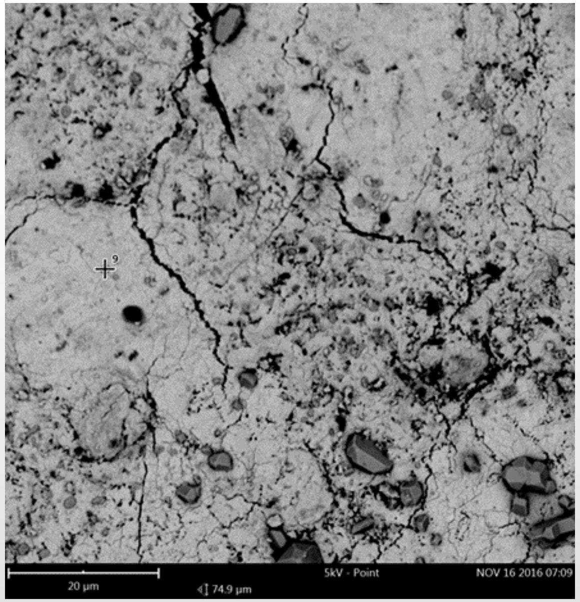


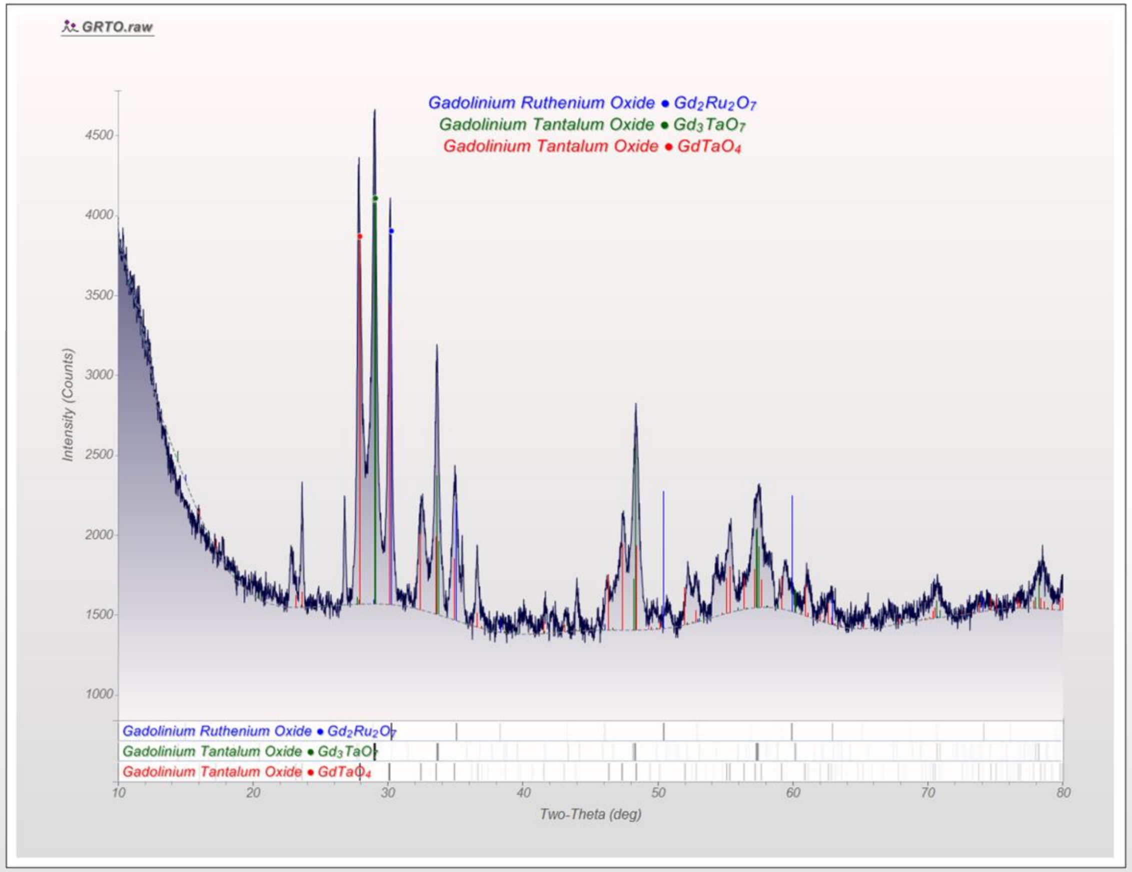


Buckingham force field:

- *Gd-Ru-O force field parameters came from Minervini, RW Grimes, KE Sickafus J Am Ceram Soc 83 (2000),*
- *Ta-O parameters came from S.M.Woodley, P.D.Battle, J.D.Gale and C.R.A.Catlow Phys. Chem. Chem. Phys., 1, 2535-2542 (1999).*

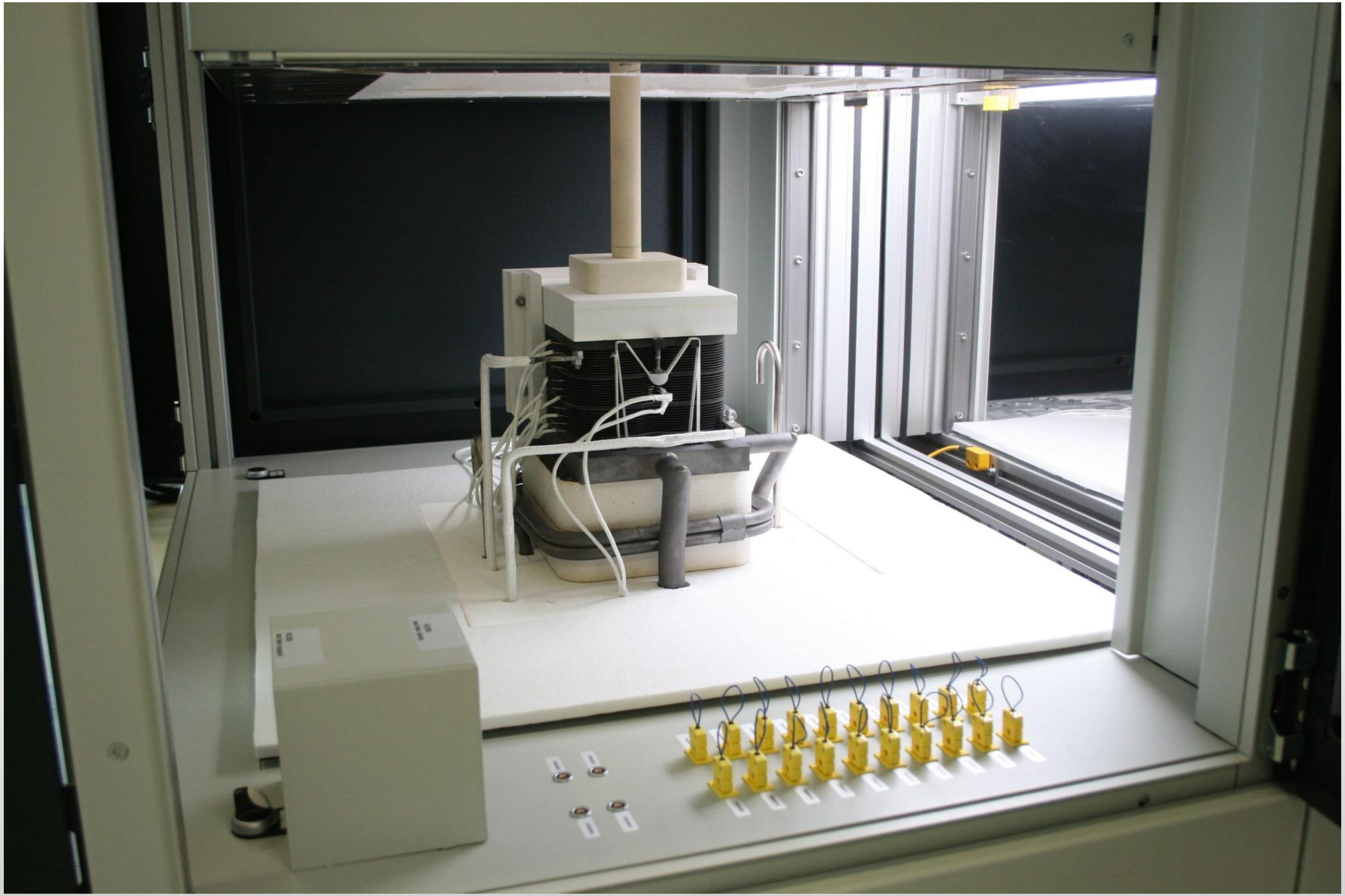






$$2Gd_2O_3 + Ta_2O_5 + 2RuO_2 \longrightarrow 2Gd_2(Ta, Ru)O_7 + \frac{1}{2} O_2$$

Solid state reaction, mechanical mixing, sintering in air, hot pressing



CONCLUSIONS

- Potential exist to harvest electrical power from excess enthalpy from gas turbine engines.

- Computational methods have enabled some fundamental parameters to be predicted in the development of thermoelectric materials.

- Some descriptions (band structure) are very sensitive to such things as mesh density.

- Oxide pyrochlores have potential as a thermoelectric materials.