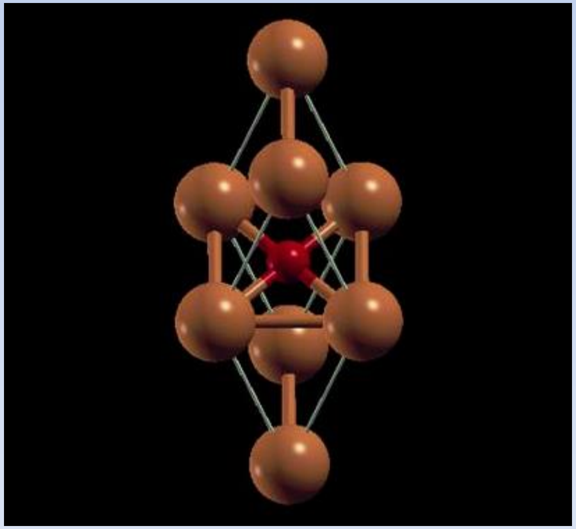
Setup

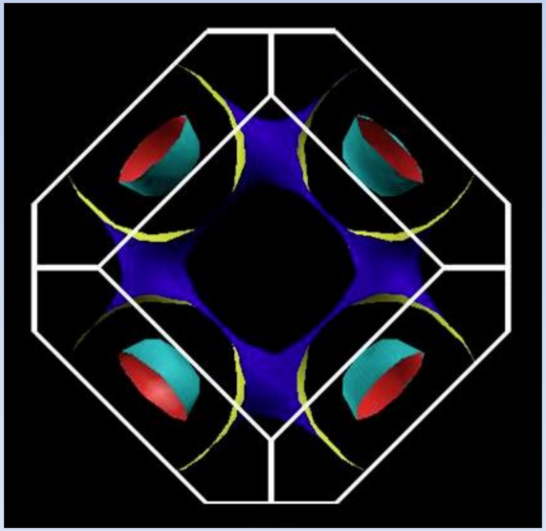
APS physics
MARCH MEETING 2015
March 2 - 6 • San Antonio

A DFT Study of Electron-Phonon Coupling in Proxy CuX (X = S, Se, Te) Structures and Its Relationship to Possible Manifestation of Superconductivity



Paul M. Grant
W2AGZ Technologies

Robert H. Hammond
Stanford University



Session Q11
Chalcogenide Superconductors
2:30 PM – 4:54 PM, Wednesday, 4 March

Paper 11
4:06 PM – 4:18 PM
Room 007B

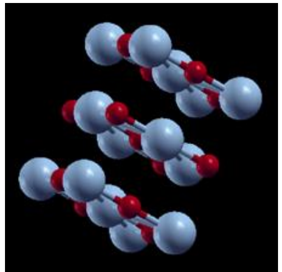
– Our Computational Tool Box –

- DFT + Hubbard U
  - Quantum Espresso
    - Fermiologies, States (DOS), Phonons, e-p “Lambda”
- Graphics
  - Xcrysden, XMGRACE
    - Fermi Surfaces, Projected DOS
- Modeling
  - Debye Temperatures a la Gibbs2 Package
    - Thanks to Alberto Otero-de-la-Rosa, http://azufre.quimica.uniovi.es/src/gibbs2/gibbs2.pdf
  - Then Superconductivity via Eliashberg/McMillan!

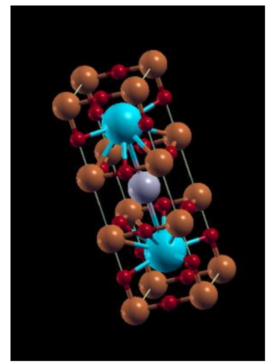
The Various Flavors of Copper "Monoxide"

- Siemons, et al. (2009)
- Grant (2008)
- Franchini Group (2011)
- Cococcioni Group (2011)

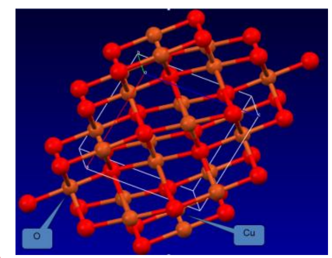
tet-rs-CuO



"1-2-3"



Tennorite



Relative Ground State Energies

Can we <u>compute/synthesize</u> the <u>S, Se, Te</u> analogues ...and what would be their physical properties wrt magnetism and superconductivity?

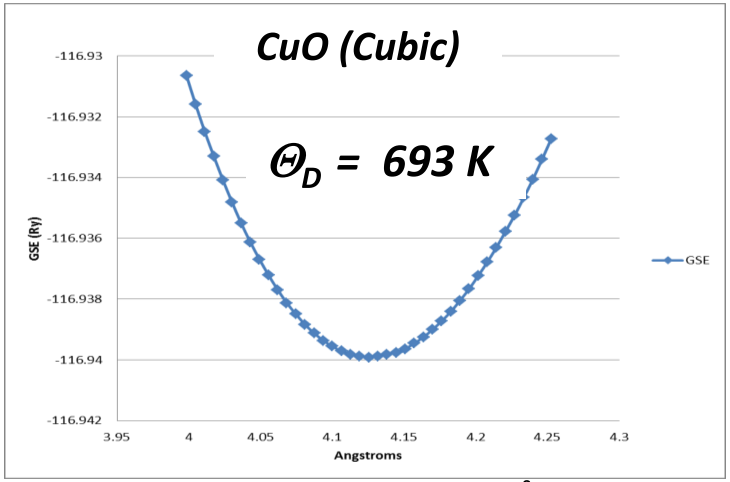
Magnetic properties revealed at APS MM Denver 2014. Now superconductivity!

"Configuration/Coordination Space"

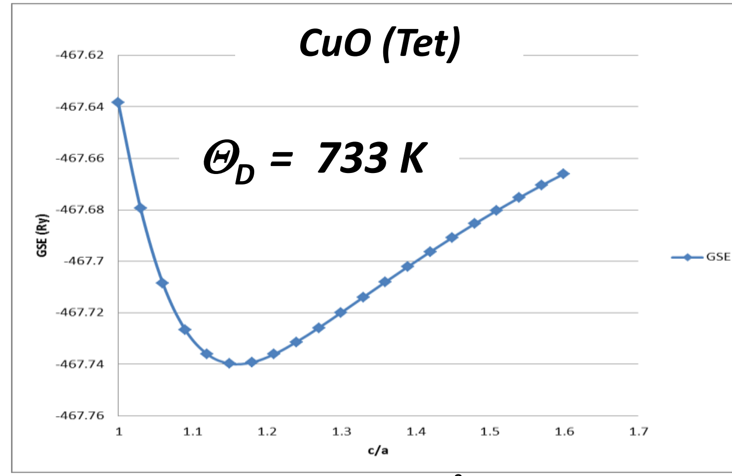
Ground State Energies via Gibbs2:

Cubic CuO & CuS *Tetragonal*

CuO

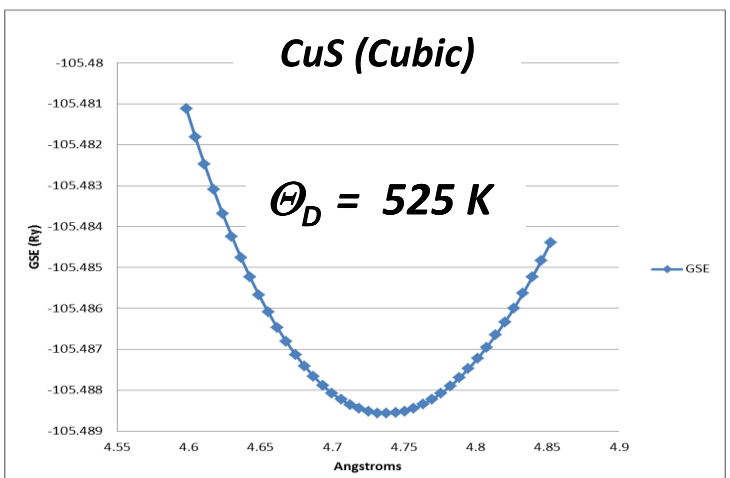


Min GSE at a0 = 4.13 Å

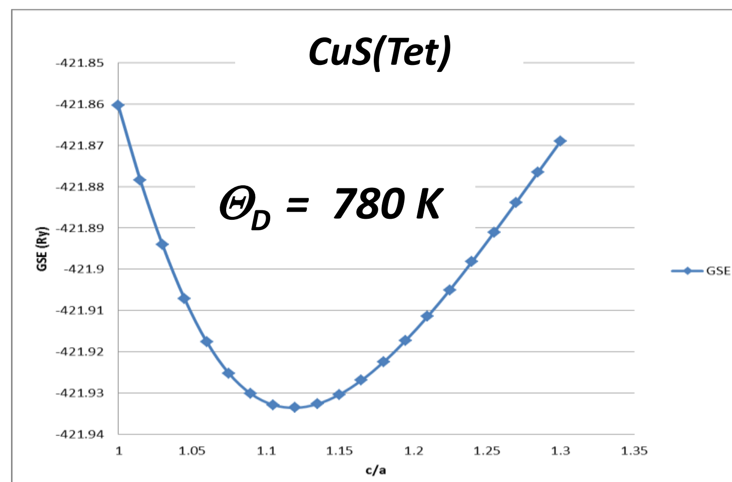


Min GSE at a0 = 3.9 Å, c/a = 1.15

CuS



Min GSE at a0 = 4.75 Å



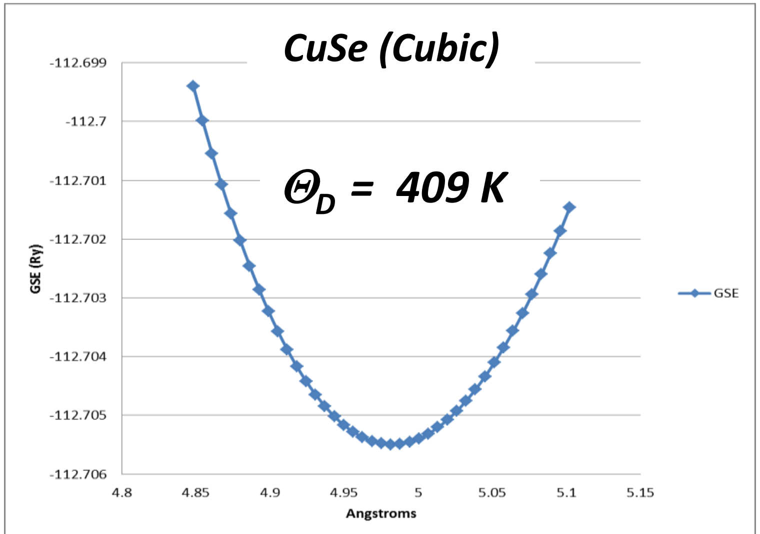
Min GSE at a0 = 4.5 Å, c/a = 1.12

Ground State Energies via Gibbs2: CuSe & CuTe

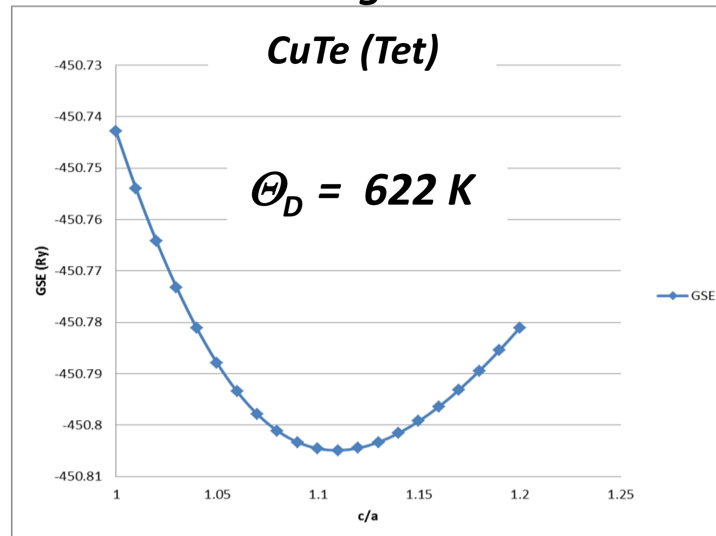
Cubic

Tetragonal

CuSe

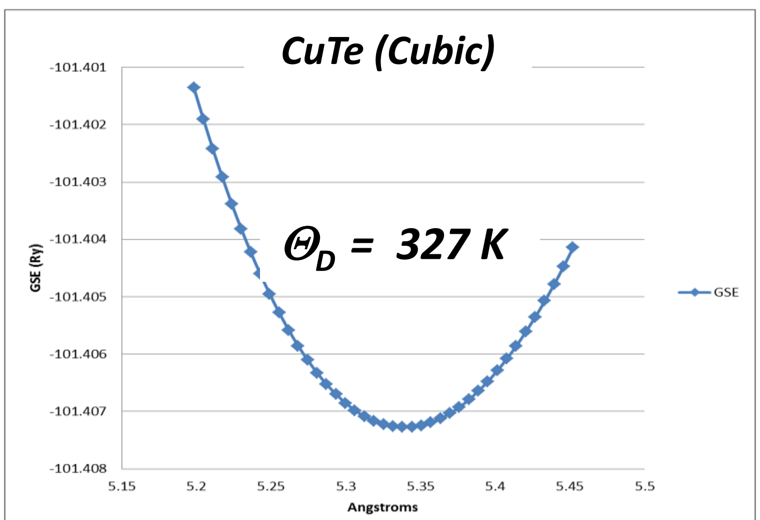


Min GSE at a0 = 5.0 Å

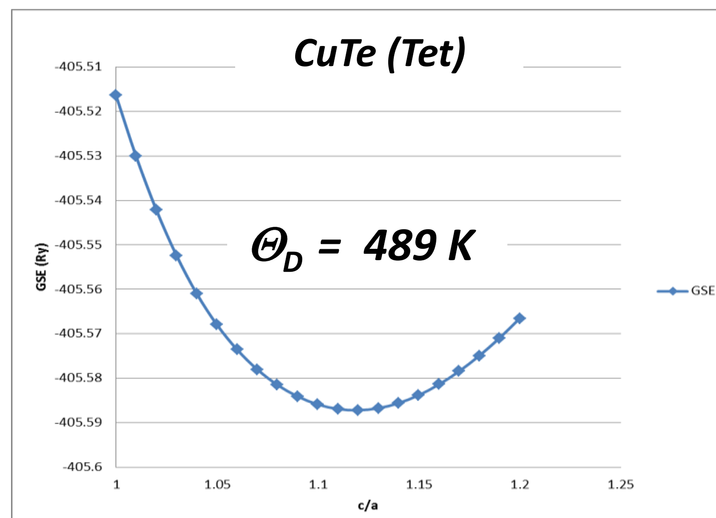


Min GSE at a0 = 4.75 Å, c/a = 1.1

CuTe



Min GSE at a0 = 5.34 Å



Min GSE at a0 = 5.05 Å, c/a = 1.1

Superconductivity and Phonons

BCS via Eliashberg-McMillan

$$H_{el-ph} = \sum_{\mathbf{k},\mathbf{q},\nu} g^{\mathbf{q}_\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}} c^{\dagger m}_{\mathbf{k}+\mathbf{q}} c^{n}_{\mathbf{k}} (b^{\dagger}_{-\mathbf{q},\nu} + b_{\mathbf{q},\nu})$$

$$\lambda_{\mathbf{q},\nu} = \frac{2}{N(\varepsilon_F)\omega_{\mathbf{q},\nu}} \sum_{mn}\sum_{\mathbf{k}} \left| g^{\mathbf{q}_\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}} \right|^2 \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F)\delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F)$$

$$\alpha^2 F(\omega) = \frac{1}{N(\varepsilon_F)} \sum_{mn}\sum_{\mathbf{q},\nu} \delta(\omega - \omega \ldots \varepsilon_F)$$

$$\lambda = 2\int_0^\infty \frac{\alpha^2 F \ldots}{\omega \ldots}$$

NB! The "double deltas" will be approximated by two Gaussians of width "sigma (σ)" whose numerical convergence is governed by imposed precision limits and basis set symmetry. Con Quidado!

To get λ, need to compute ... $g_{\mathbf{k}+\mathbf{q},\mathbf{k}}$ ... !

Eliashberg-McMillan-Allen-Dynes

$$g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}_\nu,mn} = \sqrt{h/4\pi\omega_{\mathbf{q},\nu}} \left\langle \psi_{\mathbf{k}+\mathbf{q},m} \middle| \Delta V_{KS}^{\mathbf{q},\nu} \middle| \psi_{\mathbf{k},n} \right\rangle$$

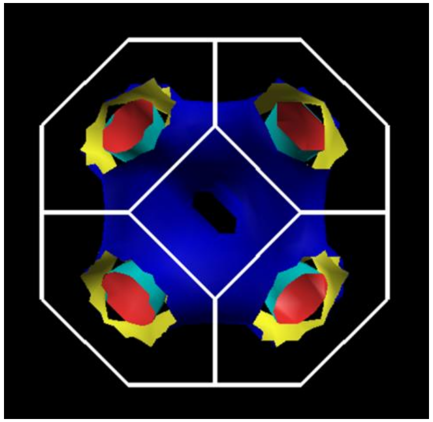
$$\Delta V_{KS}^{\mathbf{q},\nu} = \sum_{\mathbf{R}} \sum_{s} \frac{\partial V_{KS}}{\partial \vec{u}_{s,\mathbf{R}}} \cdot \vec{u}_s^{\mathbf{q},\nu} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\sqrt{N}}$$

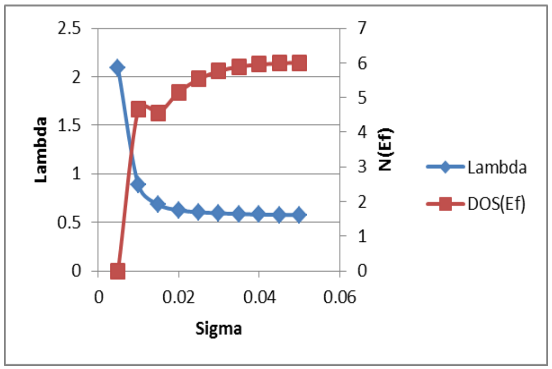
$$T_C = \frac{\Theta_{\mathrm{D}}}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right)$$

Let's Go!

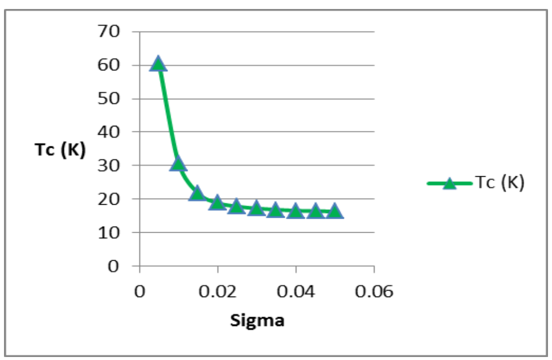
CuSe T_C

Cubic



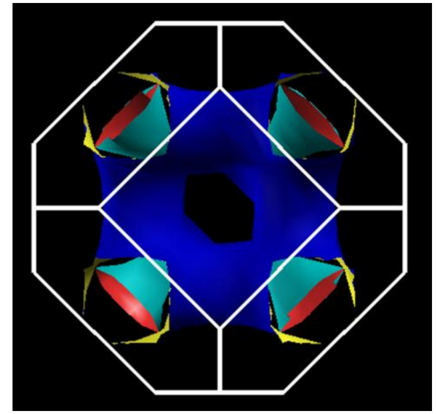


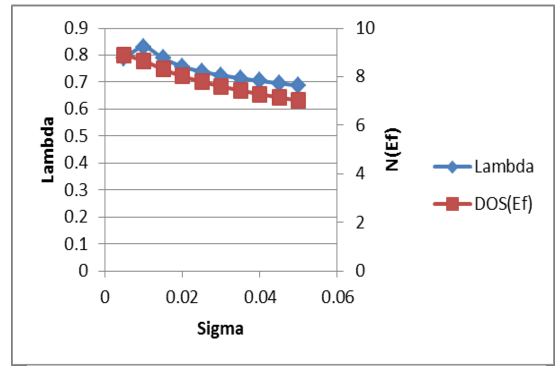
Θ_D = 409 K; μ^* = 0.0



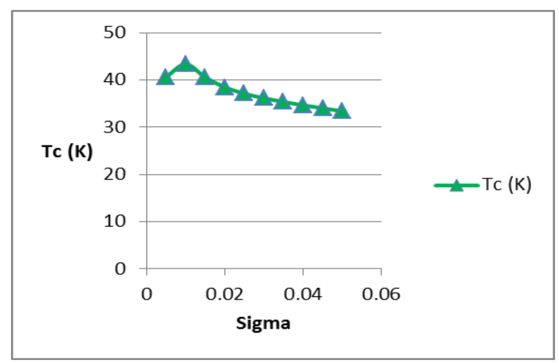
T_C(max) ~ 17 K

Tetragonal





Θ_D = 623 K; μ^* = 0.0

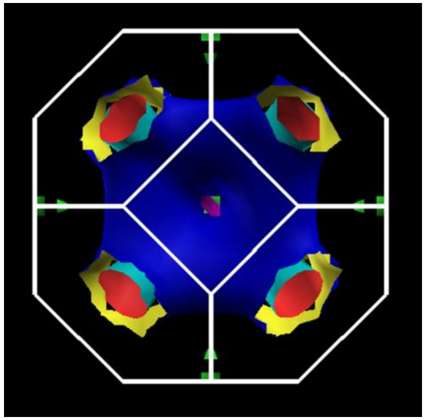


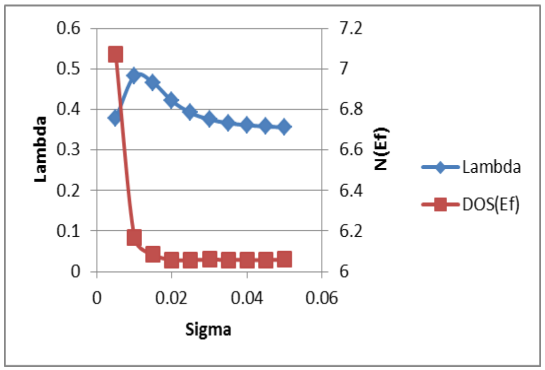
T_C(max) ~ 36 K

CuTe

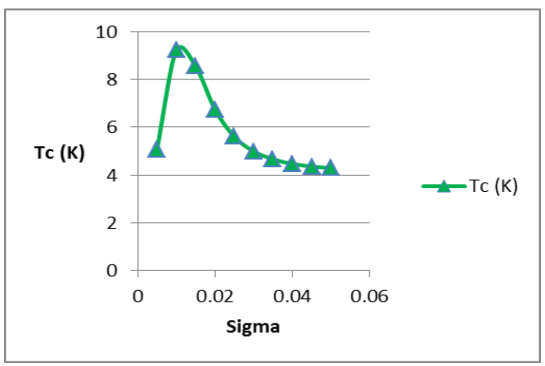
T_C

Cubic



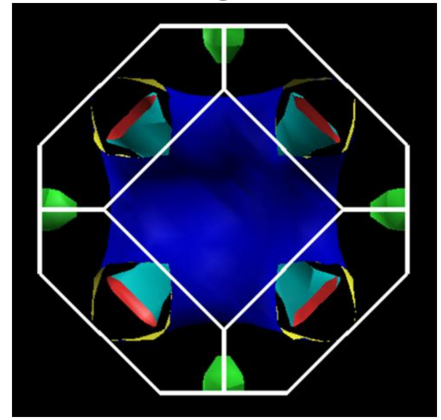


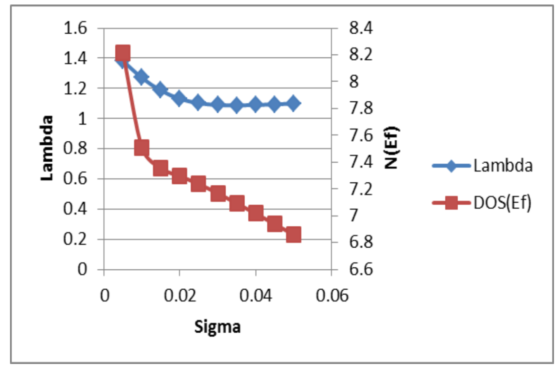
Θ_D = 327 K; μ^* = 0.0



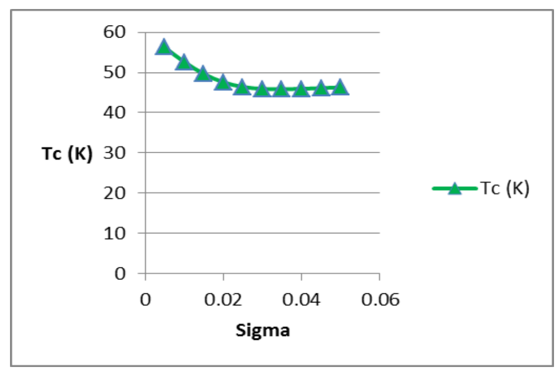
T_C(max) ~ 4.2 K

Tetragonal





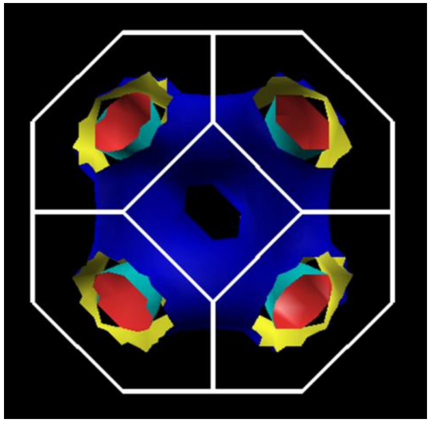
Θ_D = 490 K; μ^* = 0.0

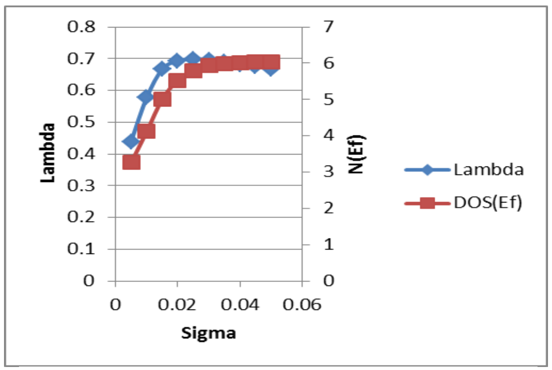


T_C(max) ~ 45 K

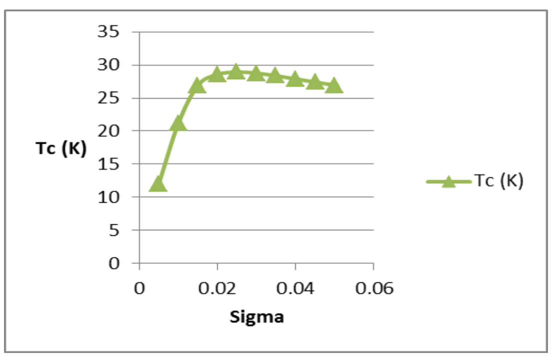
CuS T_C

Cubic



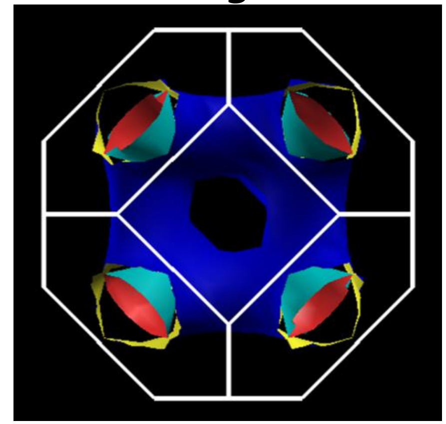


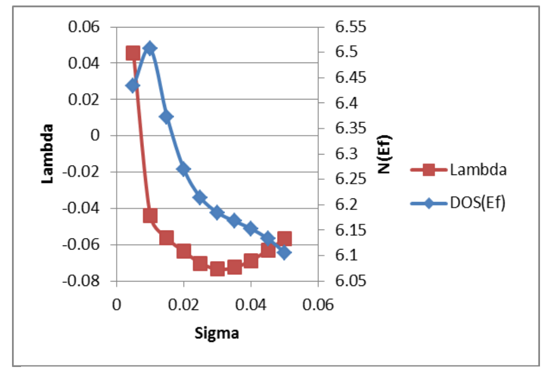
Θ_D = 525 K; μ^* = 0.0



T_C(max) ~ 28 K

Tetragonal



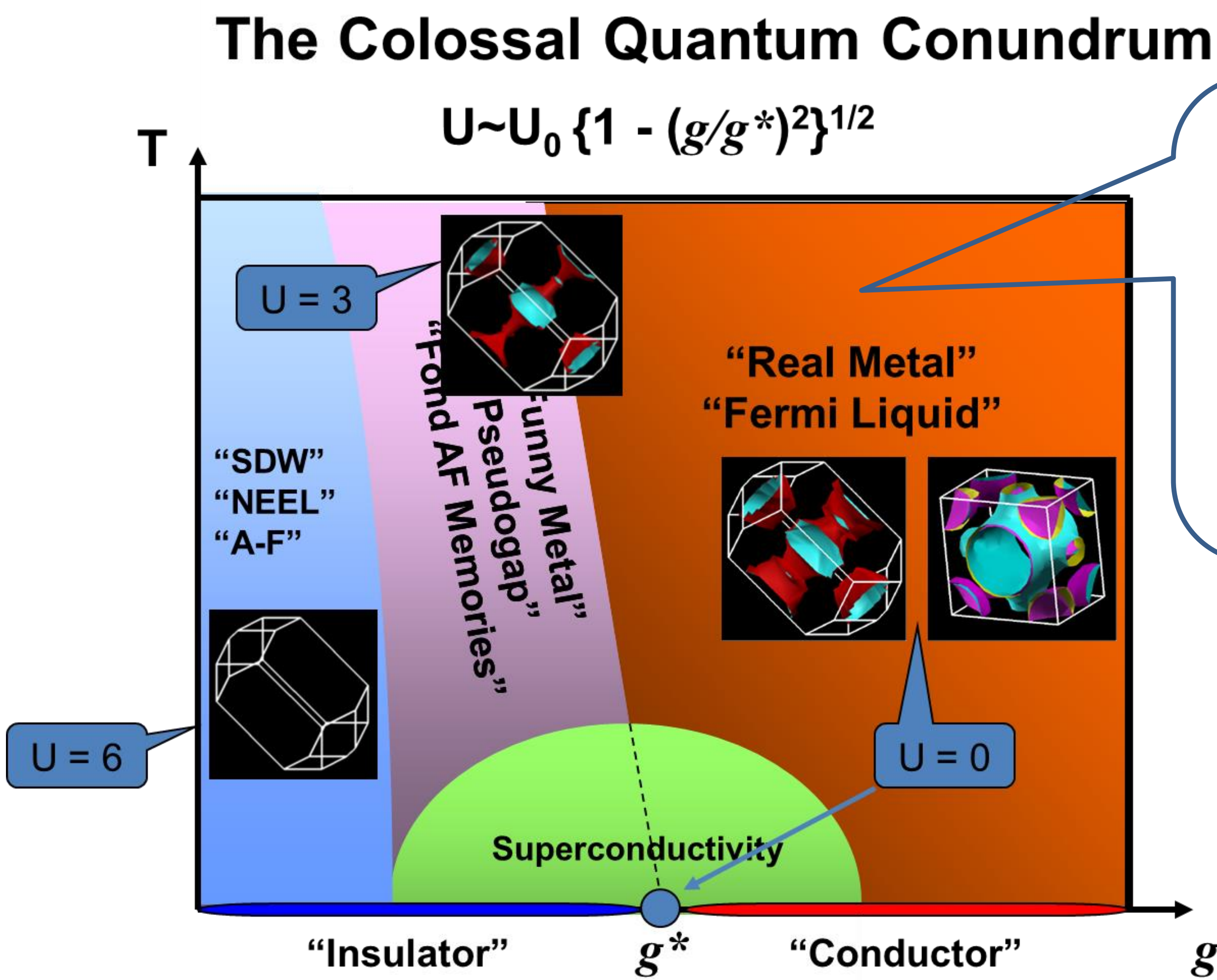


Θ_D = 780 K; μ^* = 0.0

Whoops!

- Unphysically "negative" λ !
- Convergence issues?
- Symmetry issues?
- "Needs more work ;-)"

OK…Now What About CuO? Well?



Assume a doping density for"g = 0.15 holes/CuO" in this region for experimentally determined Tet-CuO that effectively screens "U" such that we have an "ideal" Fermi liquid.

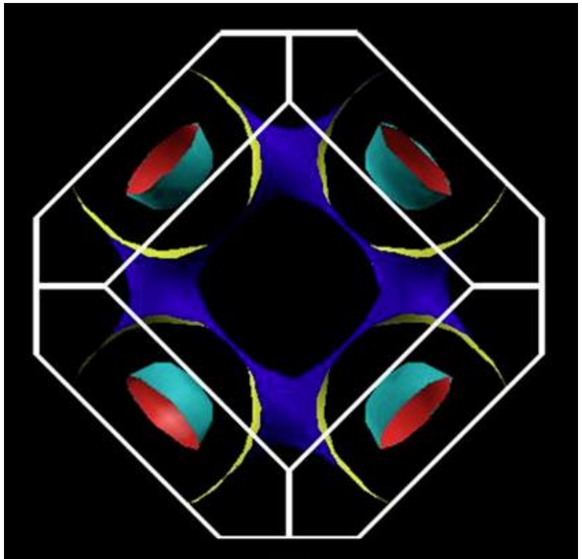
Then what does Gibbs2 and Eliashberg-McMillan tell us about the possibility of electron-phonon mediated superconducting copper oxide perovskites?

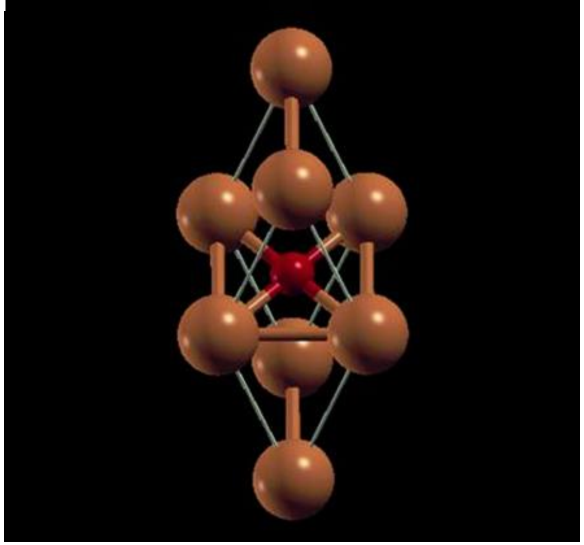
CuO

(tetragonal)

<u>q = 0.15/CuO</u>

T_c



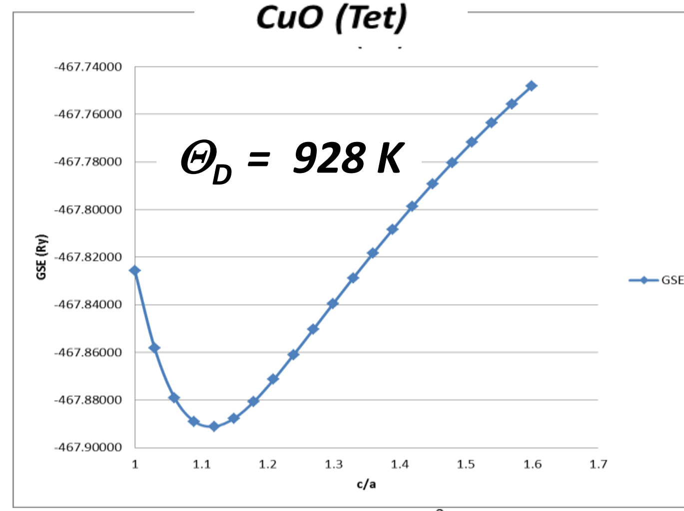


Ipso Facto...

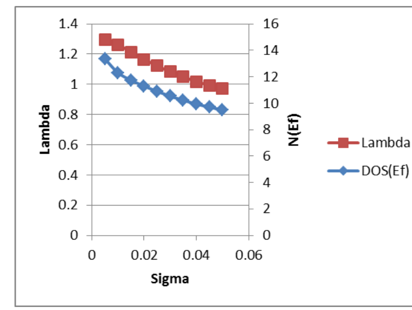
At least at optimum doping...

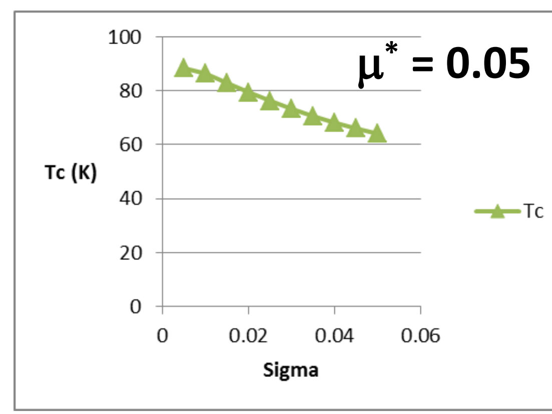
the holes are paired by lattice shakes...

with maybe a little help from their spins!



Min GSE at a0 = 3.9 Å, c/a = 1.15

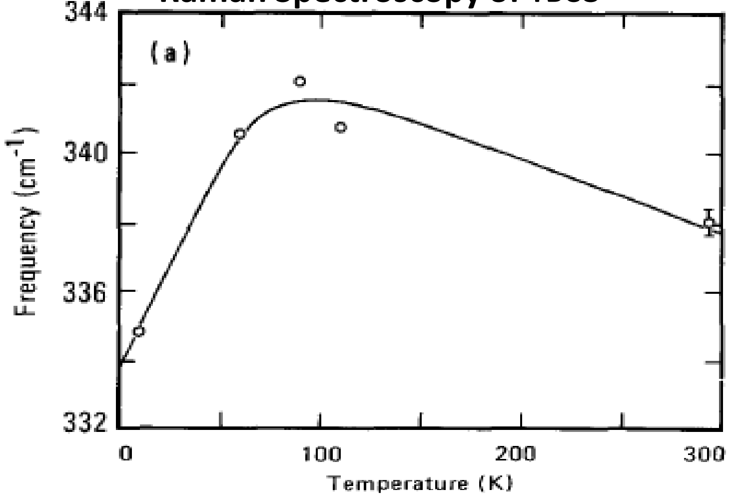




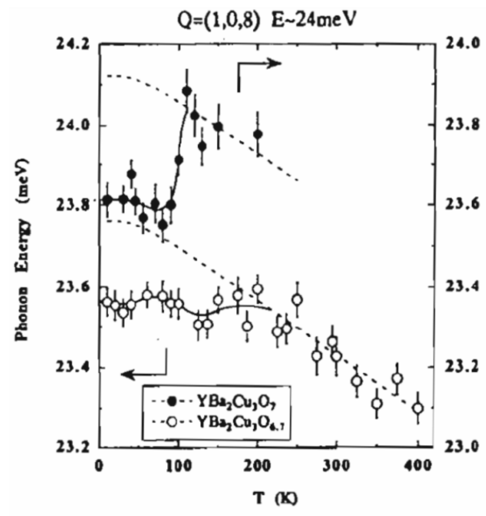
T_c(avg) ~ 75 K

So What Else is New?

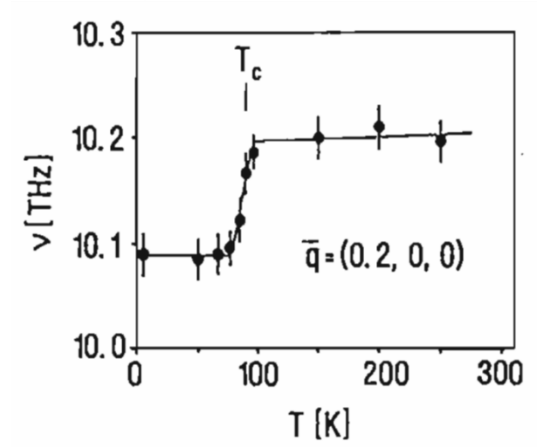
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)
Raman Spectroscopy of YBCO



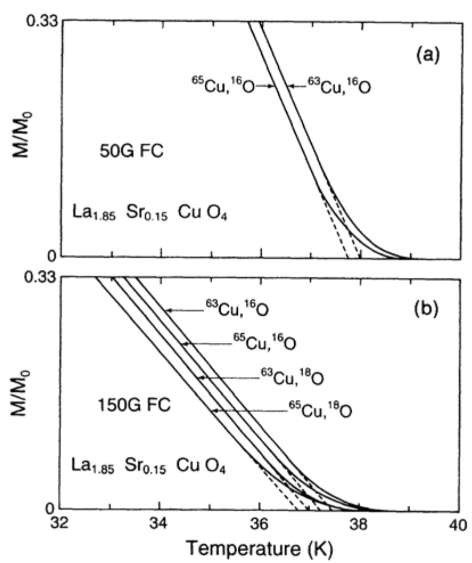
Harashima, et al., Physica C263, 257 (1996)



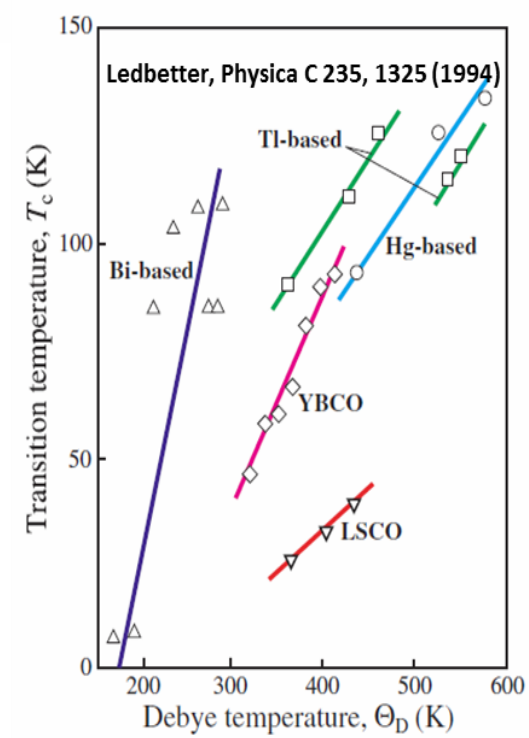
Pyka, et al., PRL 70, 1457, (1993)



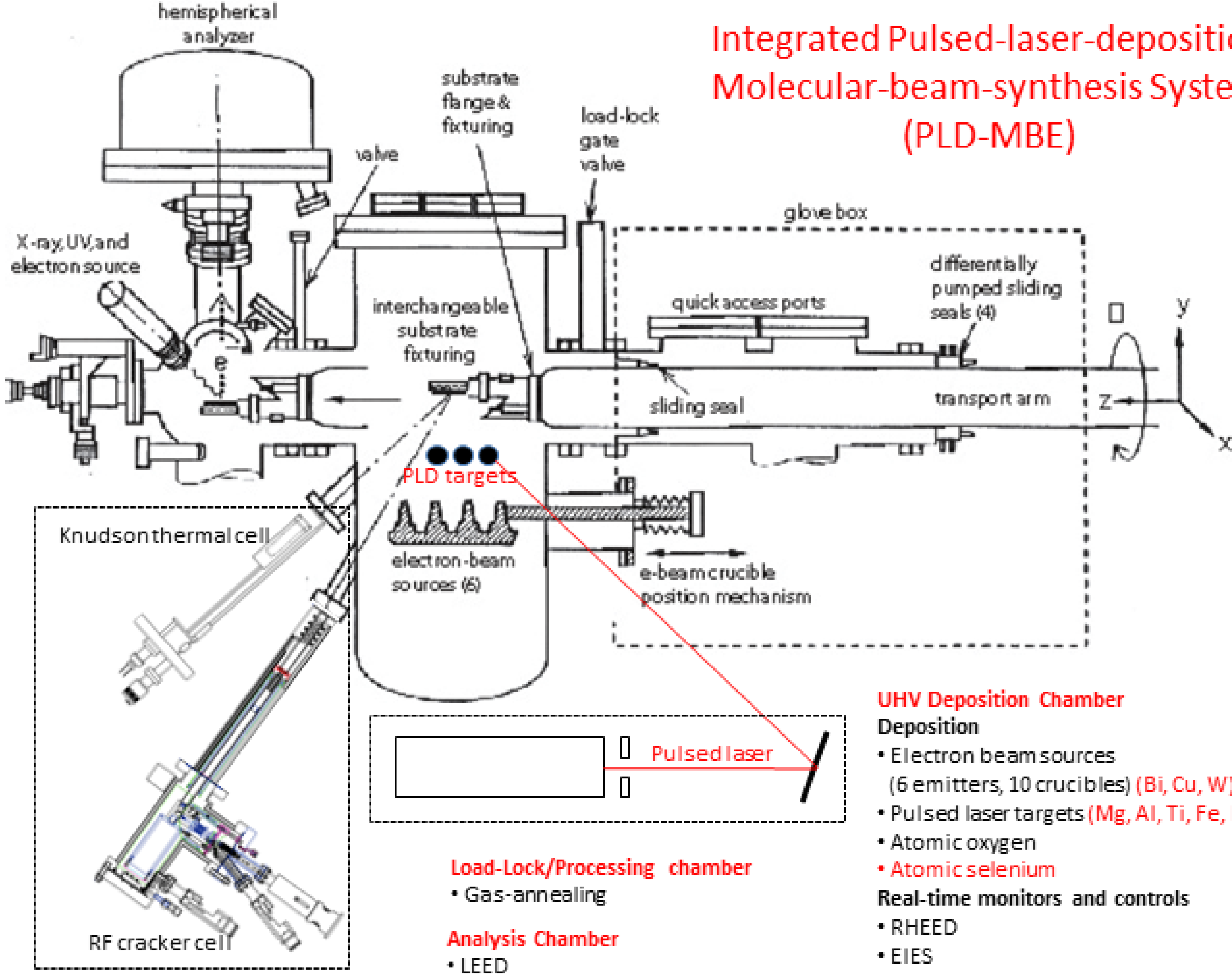
Franck, Harker, Brewer, PRL 71, (1993)
Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$



We can see Phonons have been there ever since the Creation!



At the End of the Day...
Can We Actually Make Any of this Stuff?



UHV Deposition Chamber

Deposition

- Electron beam sources (6 emitters, 10 crucibles) (Bi, Cu, W)
- Pulsed laser targets (Mg, Al, Ti, Fe, Ni)
- Atomic oxygen
- Atomic selenium

Real-time monitors and controls

- RHEED
- EIES
- QCM
- Atomic absorption rate control

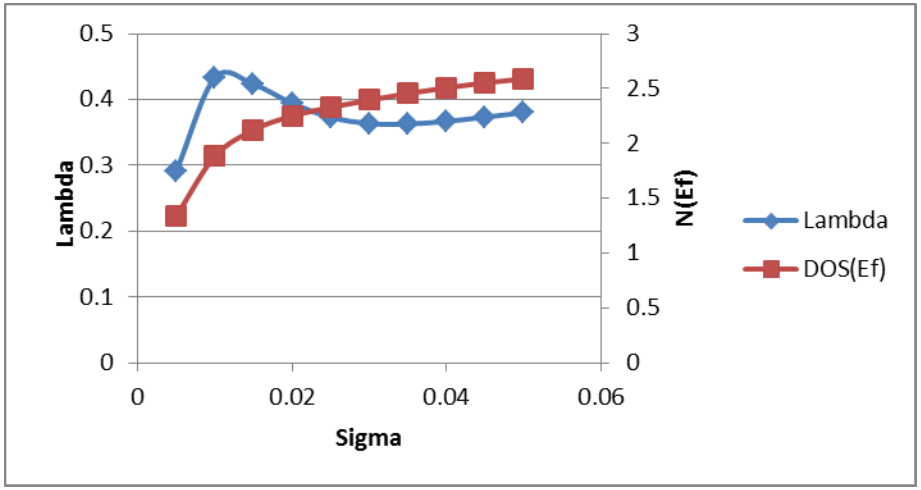
Load-Lock/Processing chamber

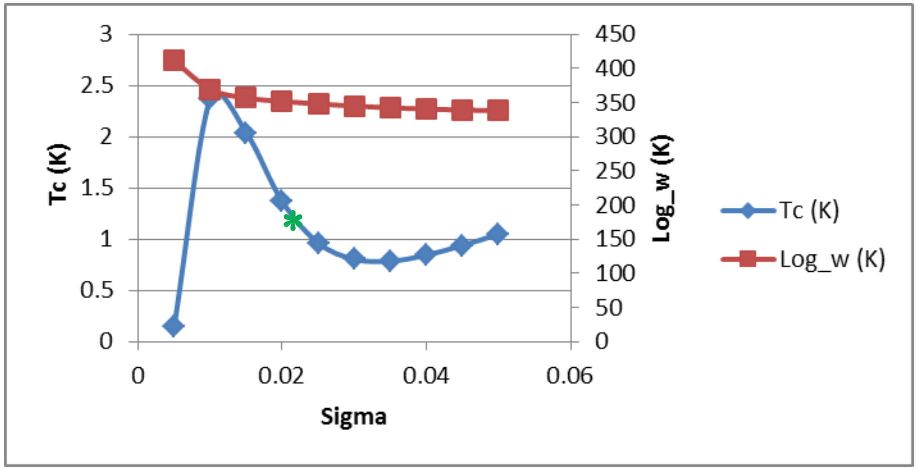
- Gas-annealing

Analysis Chamber

- LEED
- XPS
- UPS

Aluminum
(Quantum-ESPESSO Example)





μ^* = 0.1

Log_w ~ Θ_D

T_C(exp) = 1.2 K