

# Electron-Phonon Interaction in the Polymeric Superconductor, Polysulfur Nitride, $(SN)_x$

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IBM Research Staff Member, Emeritus

Session P8: Focus Session: Novel Superconductors:  
Miscellaneous Materials

2007 APS March Meeting

Talk P8.00007, 12:39 PM - 12:51 PM

Wednesday, 7 March, CCC Korbel 1C

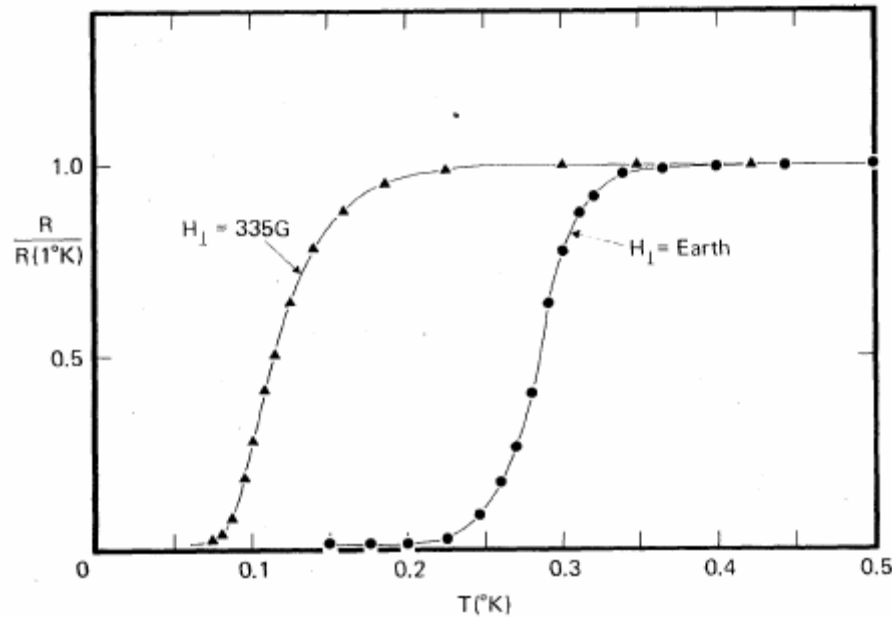
Denver, Colorado



<http://www.w2agz.com/snxaps07.htm>

# 1975: Superconductivity Discovered at 300 degrees in Polysulfurnitride, (SN)<sub>x</sub>

*...but the units are in millikelvin!*



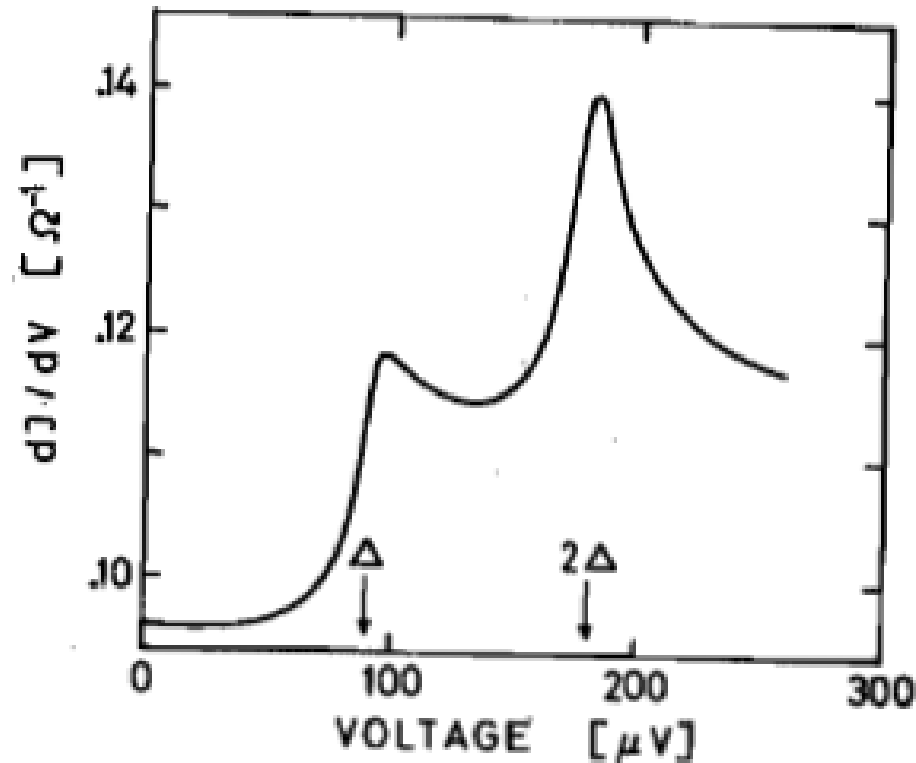
Superconductivity in Polysulfur Nitride (SN)<sub>x</sub>

R. L. Greene and G. B. Street  
IBM Research Laboratory, San Jose, California 95193

and

L. J. Suter\*†  
Department of Physics, Stanford University, Stanford, California 94305  
(Received 27 January 1975)

# Precursor to a Nobel Prize



## Tunneling Investigation of Superconducting $(SN)_x$

G. Binnig and H.E. Hoenig

Physikalisches Institut der Universität Frankfurt, Germany

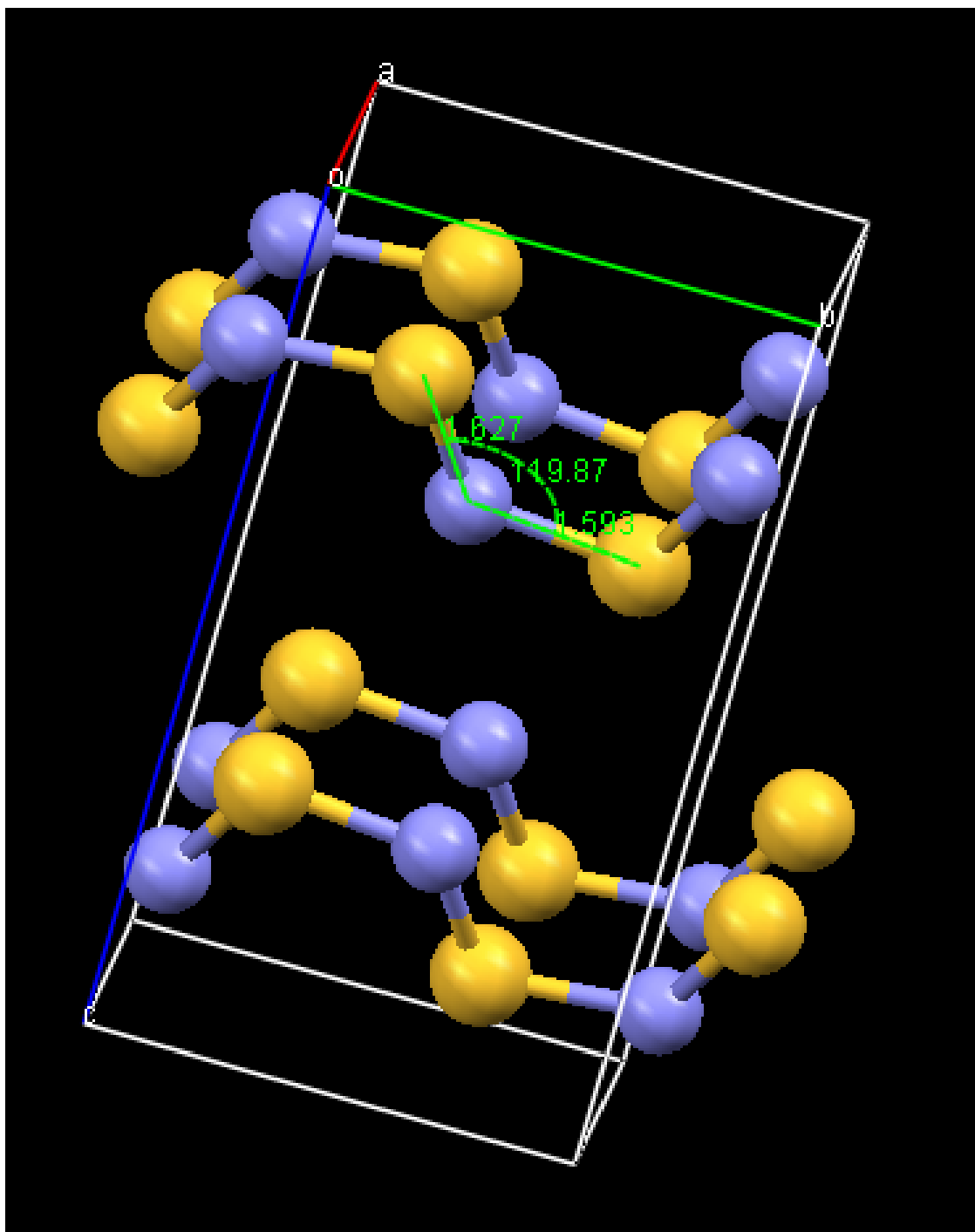
Z. Physik B 32, 23–26 (1978)

"Thanks," "Grazie," & "Hvala Lepa" to...

- Paolo Giannozzi and his team at CNR-INFN-Democritos for developing and supporting PWscf and Quantum-Espresso
- Anton Kokalj of the Jozef Stefan Institute, Slovenia, for PWgui and XCrySDen
- The UK Cambridge crystal structure data base team for developing and support of the Mercury crystal imaging package

...and all this for free!

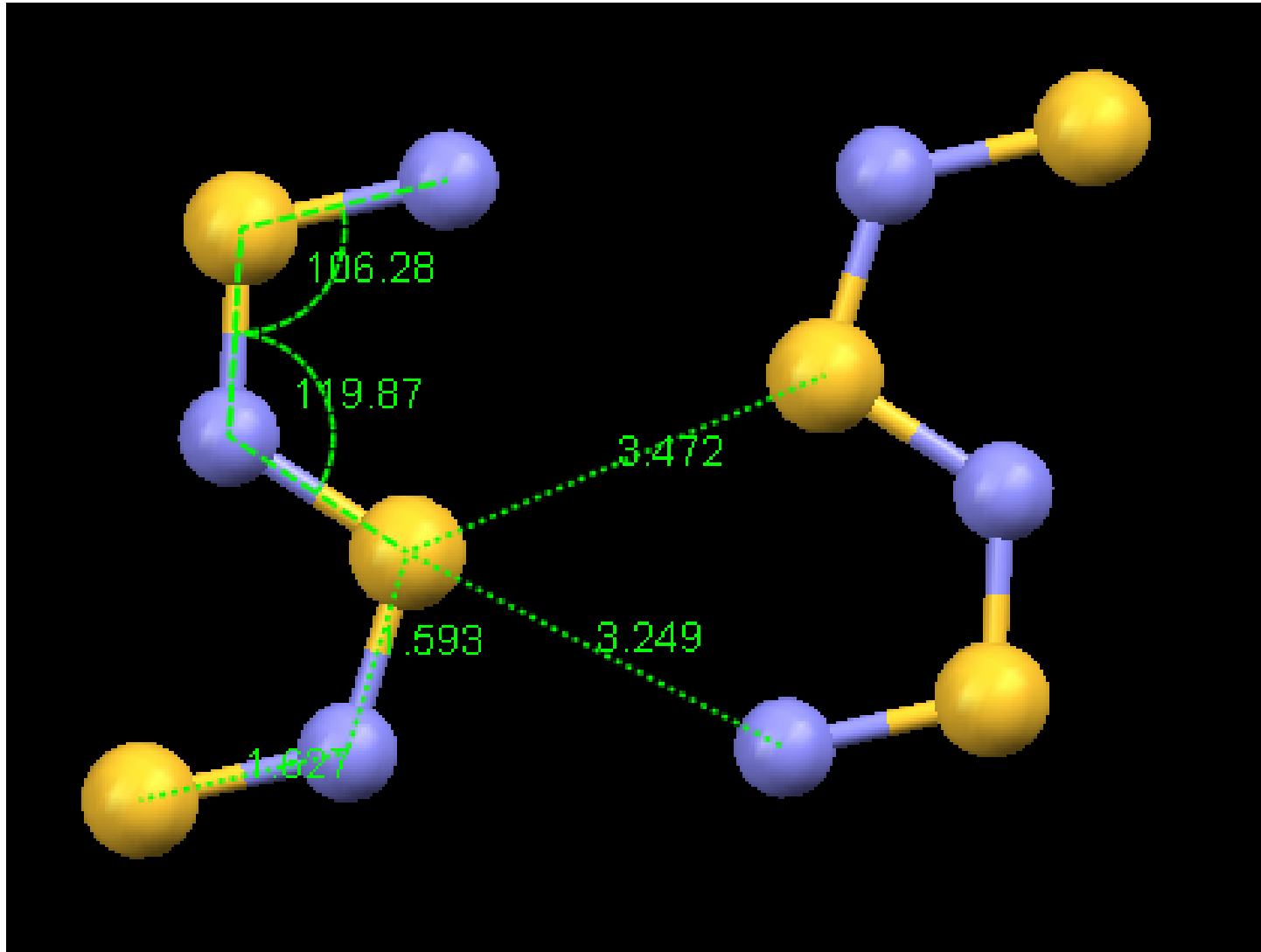
A paradigm for a future world order?

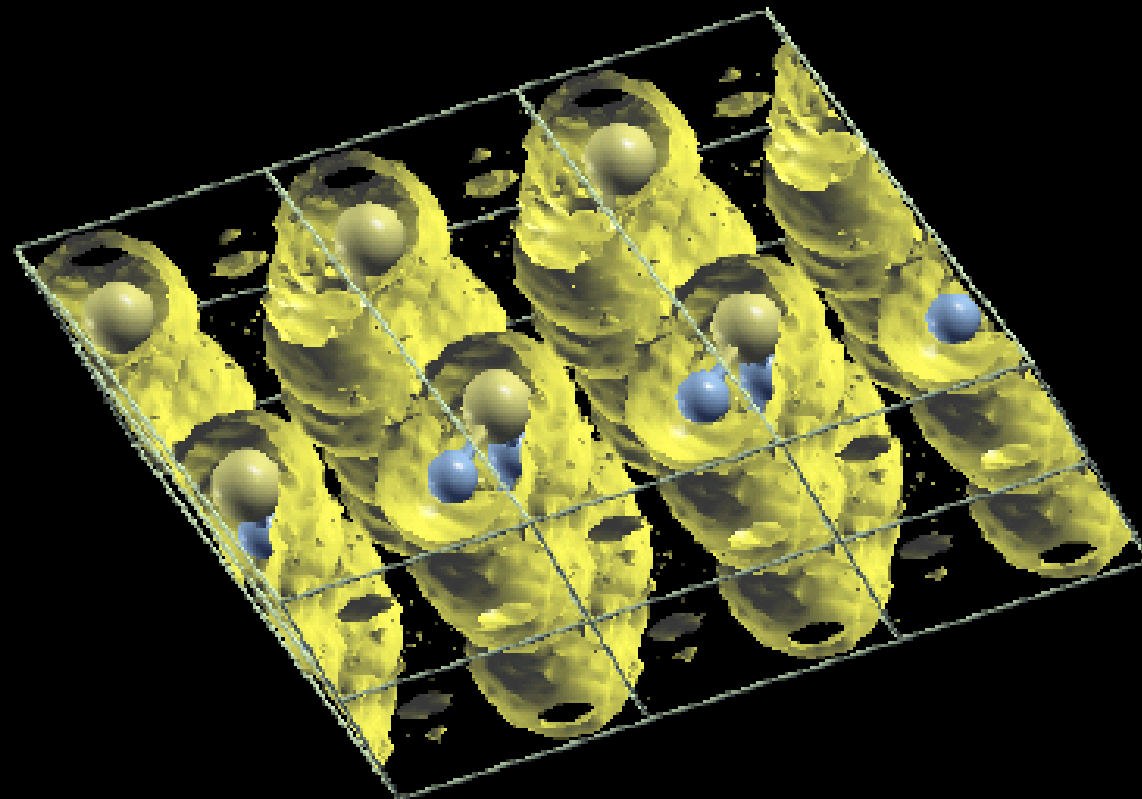


## Structure of $(\text{SN})_x$

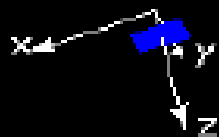
Cohen, et al., JACS 98,  
3844 (1976)

- Monoclinic  $P2_1/c$
- $a=4.485$ ,  $b=3.767$ ,  
 $c=8.452$ ,  $\beta=106.43$
- 4 N, 4 S, 2 chains
- $S=32.06$ ,  $N=14.007$
- $S[\text{Ne}]3s^23p^4$ ,  
 $N[\text{He}]2s^22p^3$
- 44 electrons
- 22+ bands
- Many phonon IRs (12-24)

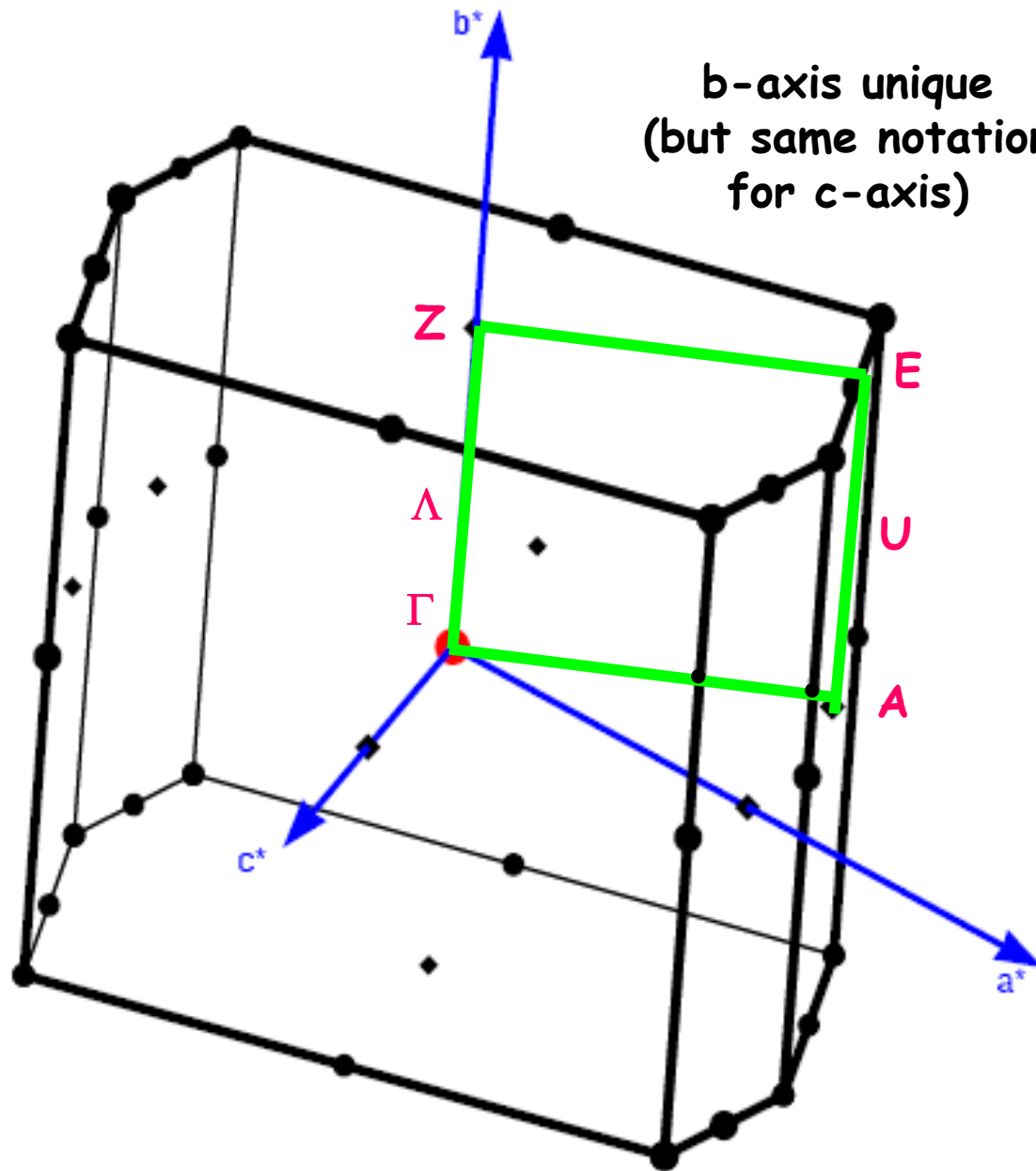




b-axis unique

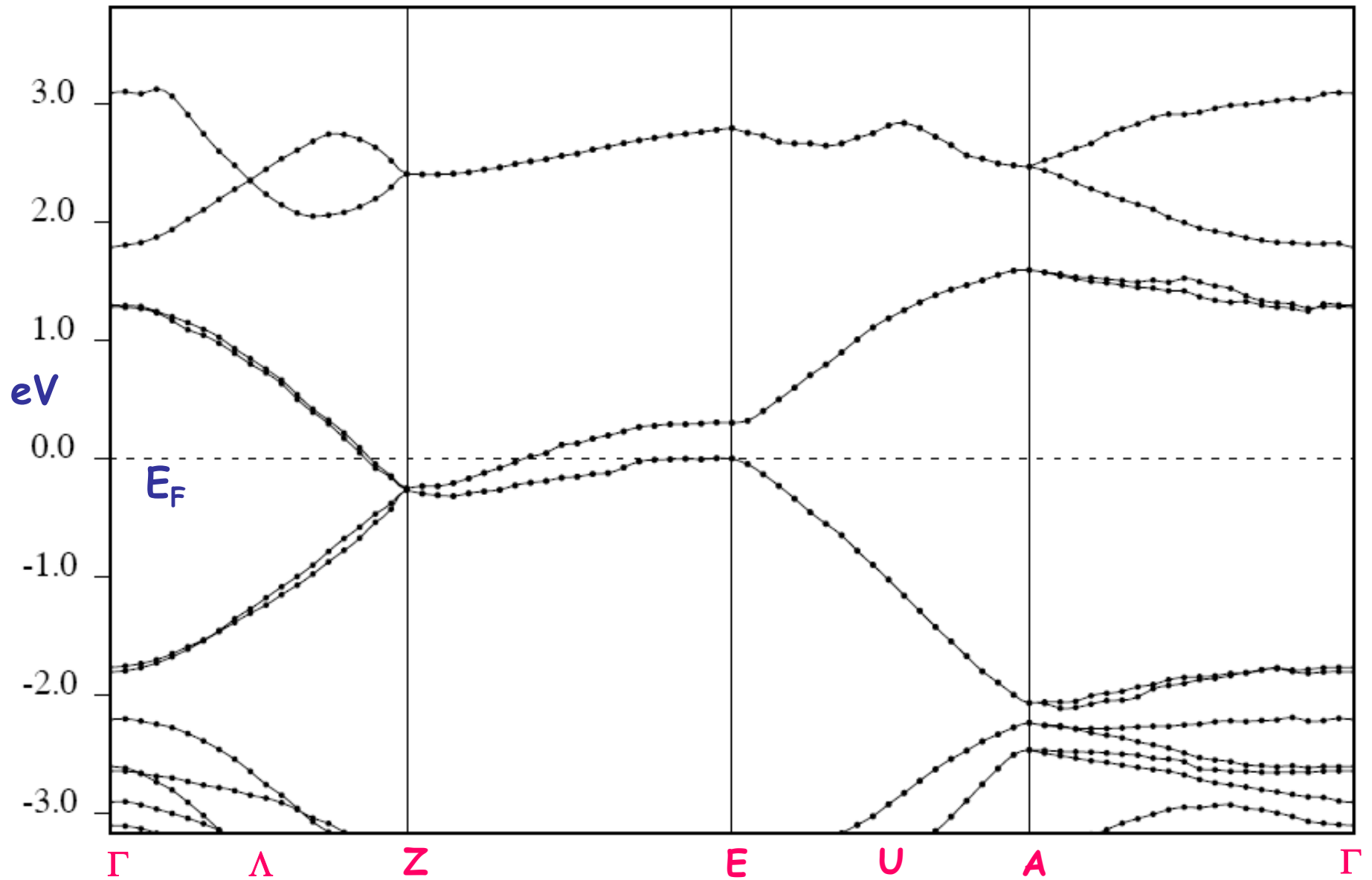


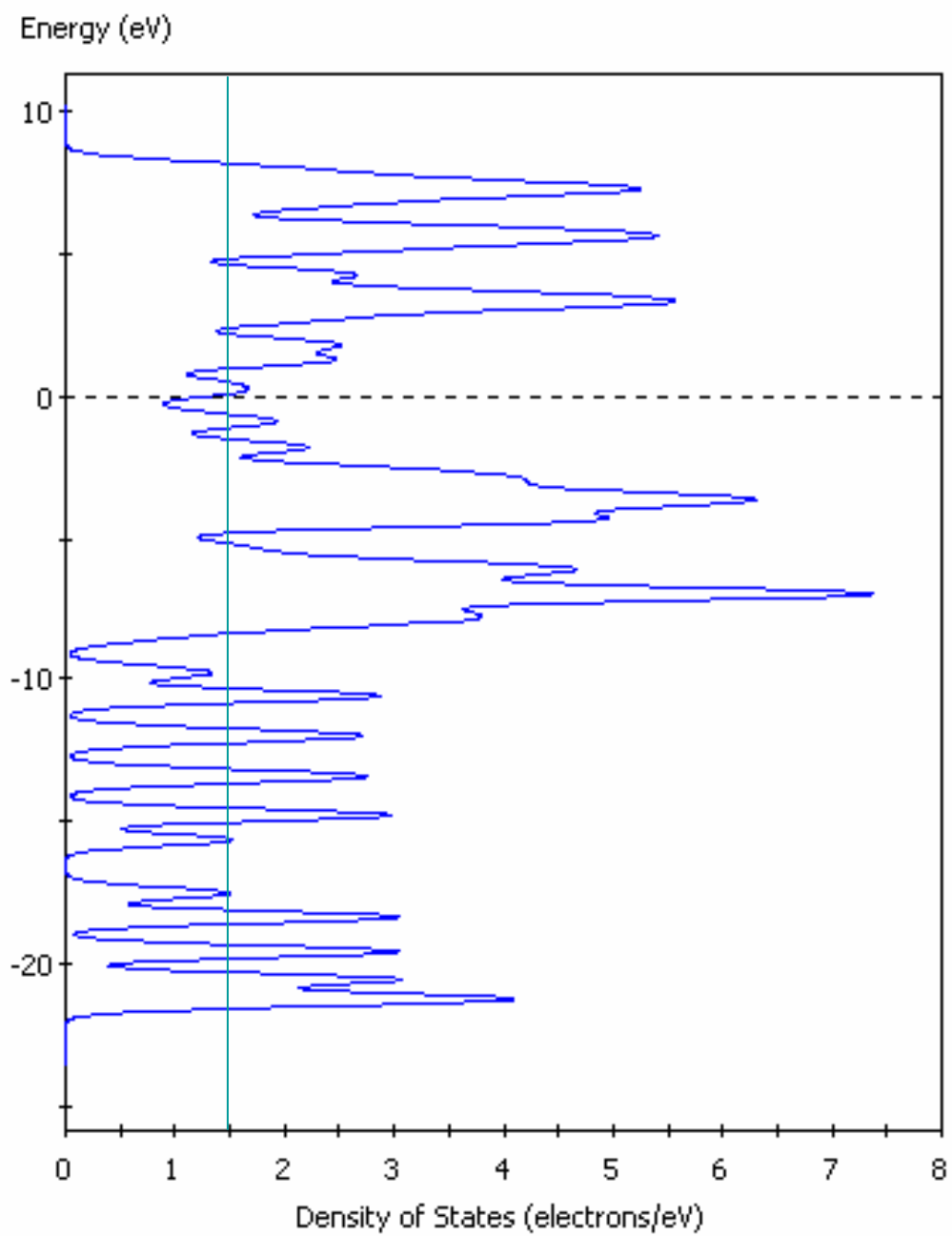
b-axis unique  
(but same notation  
for c-axis)

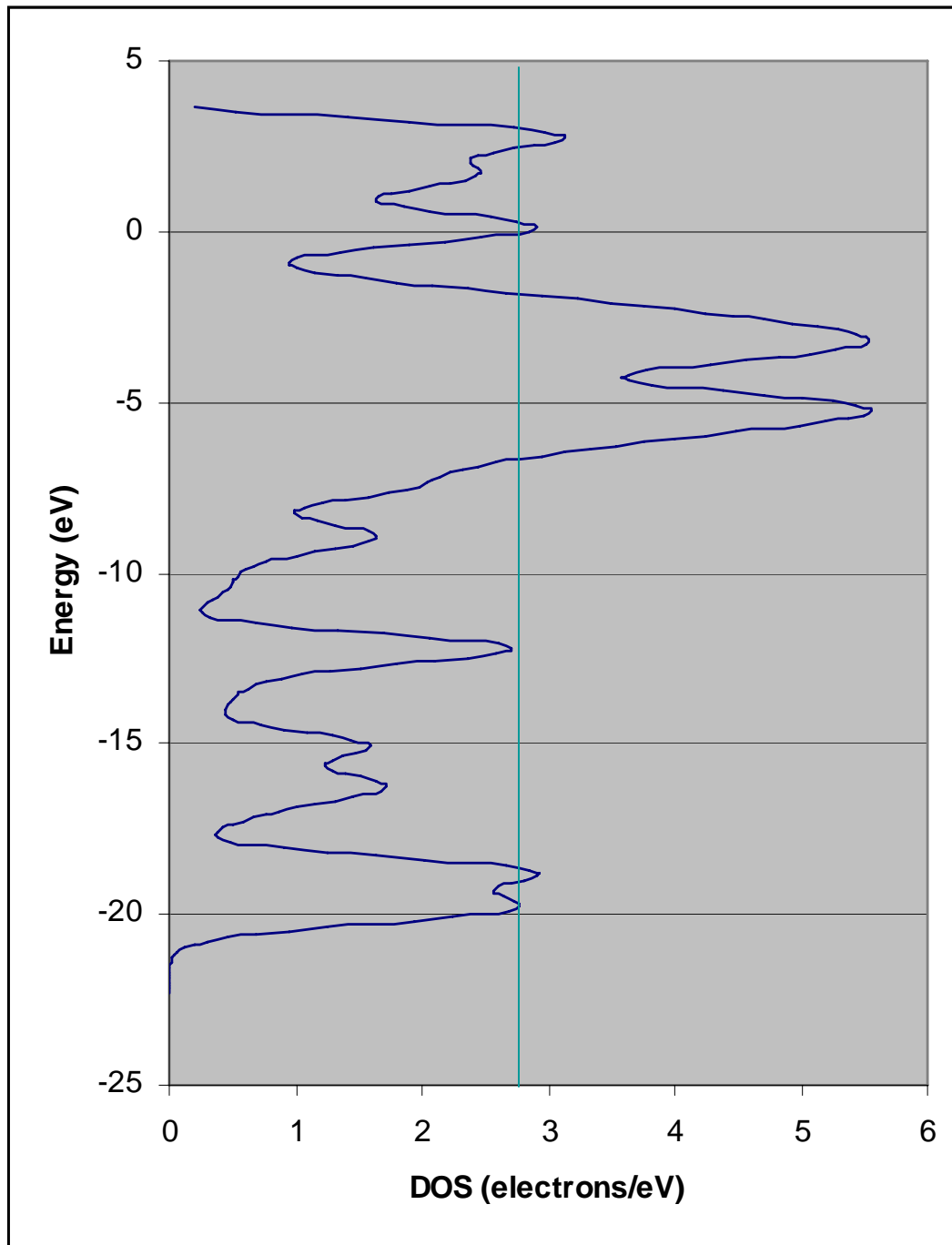


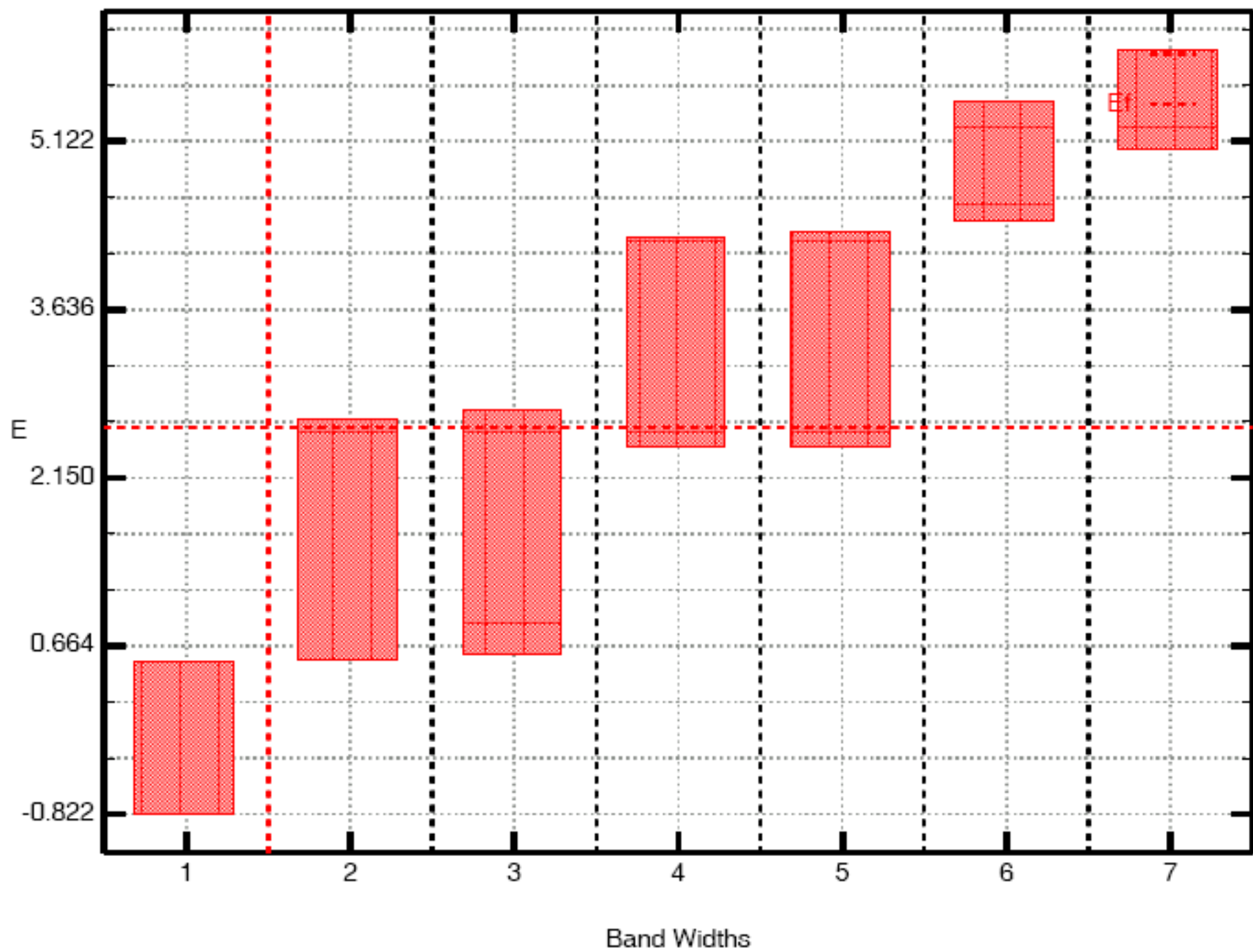


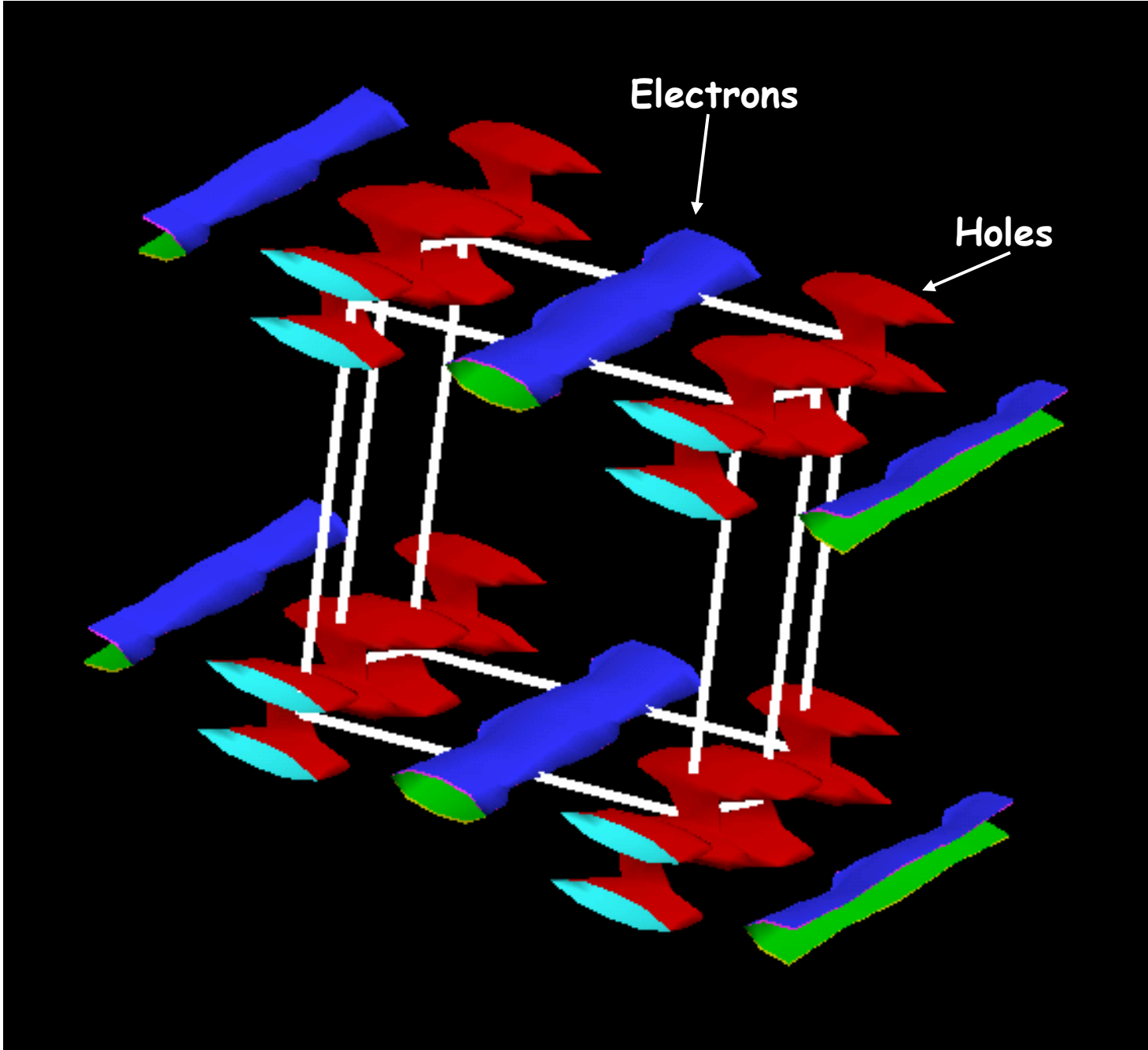
# Band Structure of (SN)<sub>x</sub>











# Electron-Phonon Coupling

$$H_{el-ph} = \sum_{\mathbf{k}q\nu} g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn} c_{\mathbf{k}+\mathbf{q}}^{\dagger m} c_{\mathbf{k}}^n (b_{-\mathbf{q}\nu}^{\dagger} + b_{\mathbf{q}\nu}) \quad (1)$$

$$\alpha^2 F(\omega) = \frac{1}{N(\epsilon_F)} \sum_{mn} \sum_{q\nu} \delta(\omega - \omega_{q\nu}) \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn}|^2 \times \delta(\epsilon_{\mathbf{k}+\mathbf{q},m} - \epsilon_F) \delta(\epsilon_{\mathbf{k},n} - \epsilon_F), \quad (2)$$

$$\lambda = 2 \int \frac{\alpha^2 F(\omega)}{\omega} d\omega = \sum_{q\nu} \lambda_{q\nu}, \quad (3)$$

$$\lambda_{q\nu} = \frac{2}{N(\epsilon_F)\omega_{q\nu}} \sum_{mn} \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{q\nu,mn}|^2 \times \delta(\epsilon_{\mathbf{k}+\mathbf{q},m} - \epsilon_F) \delta(\epsilon_{\mathbf{k},n} - \epsilon_F). \quad (4)$$

$$\gamma_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{mn} \sum_{\mathbf{k}} |g_{\mathbf{k}+\mathbf{q},\mathbf{k}}^{\mathbf{q}\nu,mn}|^2 \times \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F) \delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F) \quad (5)$$

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(\varepsilon_F)} \sum_{\mathbf{q}\nu} \frac{\gamma_{\mathbf{q}\nu}}{\omega_{\mathbf{q}\nu}} \delta(\omega - \omega_{\mathbf{q}\nu}), \quad (6)$$

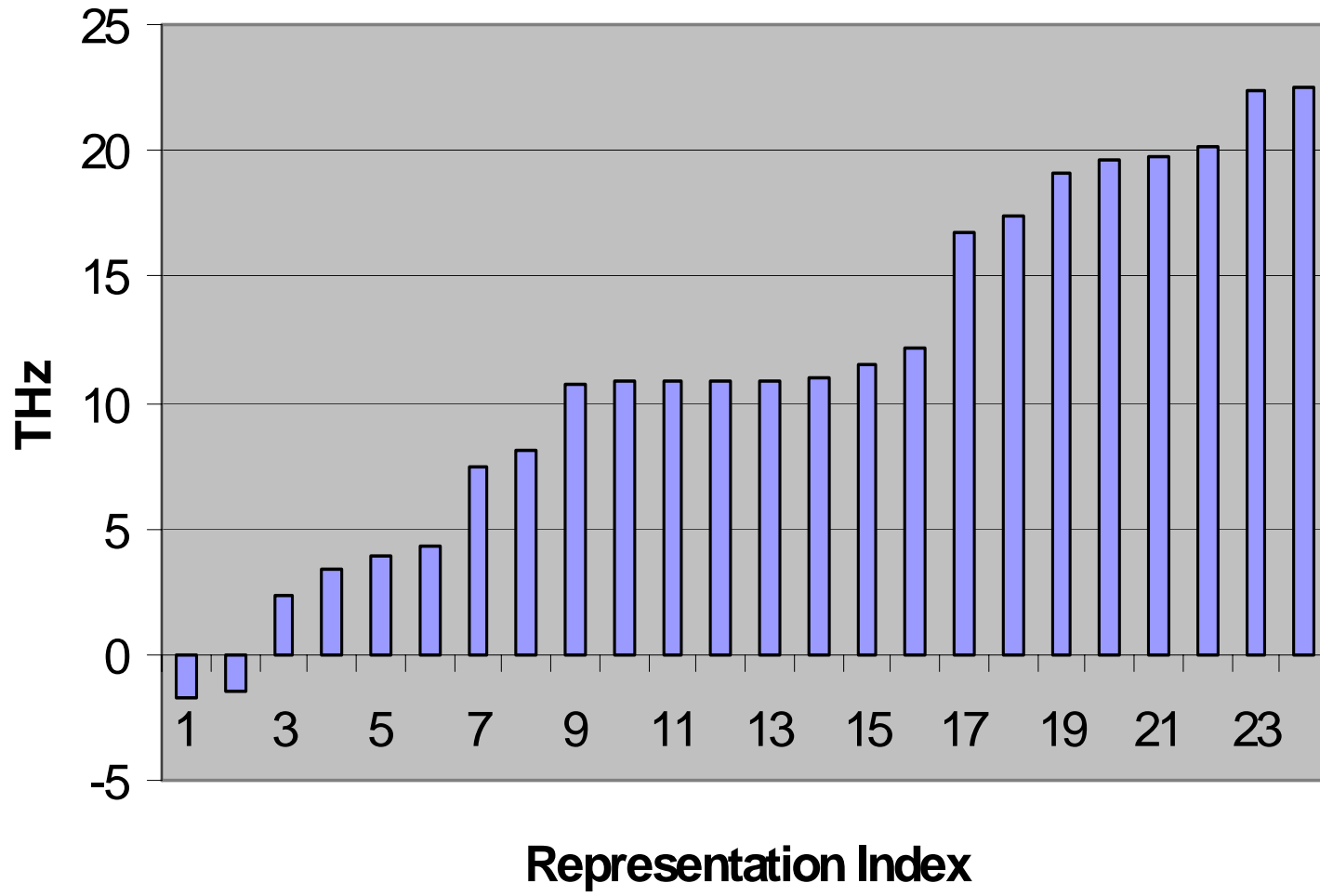
$$\lambda_{\mathbf{q}\nu} = \frac{\gamma_{\mathbf{q}\nu}}{\pi N(\varepsilon_F) \omega_{\mathbf{q}\nu}^2}. \quad (7)$$

# "Experimental Apparatus"

- Linux box running SUSE 10.1
- Dual Xeon (1.2 GHz) Motherboard, 2 GB RAM, 133 MHz FSB, Vintage ca. 2003
- Democritos Quantum Espresso Package
  - Vanderbilt US pseudopotentials for N & S
  - pw.x, 4x4x4 MP grid
  - ph.x,  $\text{tr2\_ph} = 1e-11 |\text{ddv\_scf}|^2$
  - 1 q-point => 25 hours wall time
  - Still not a fully converged calculation!

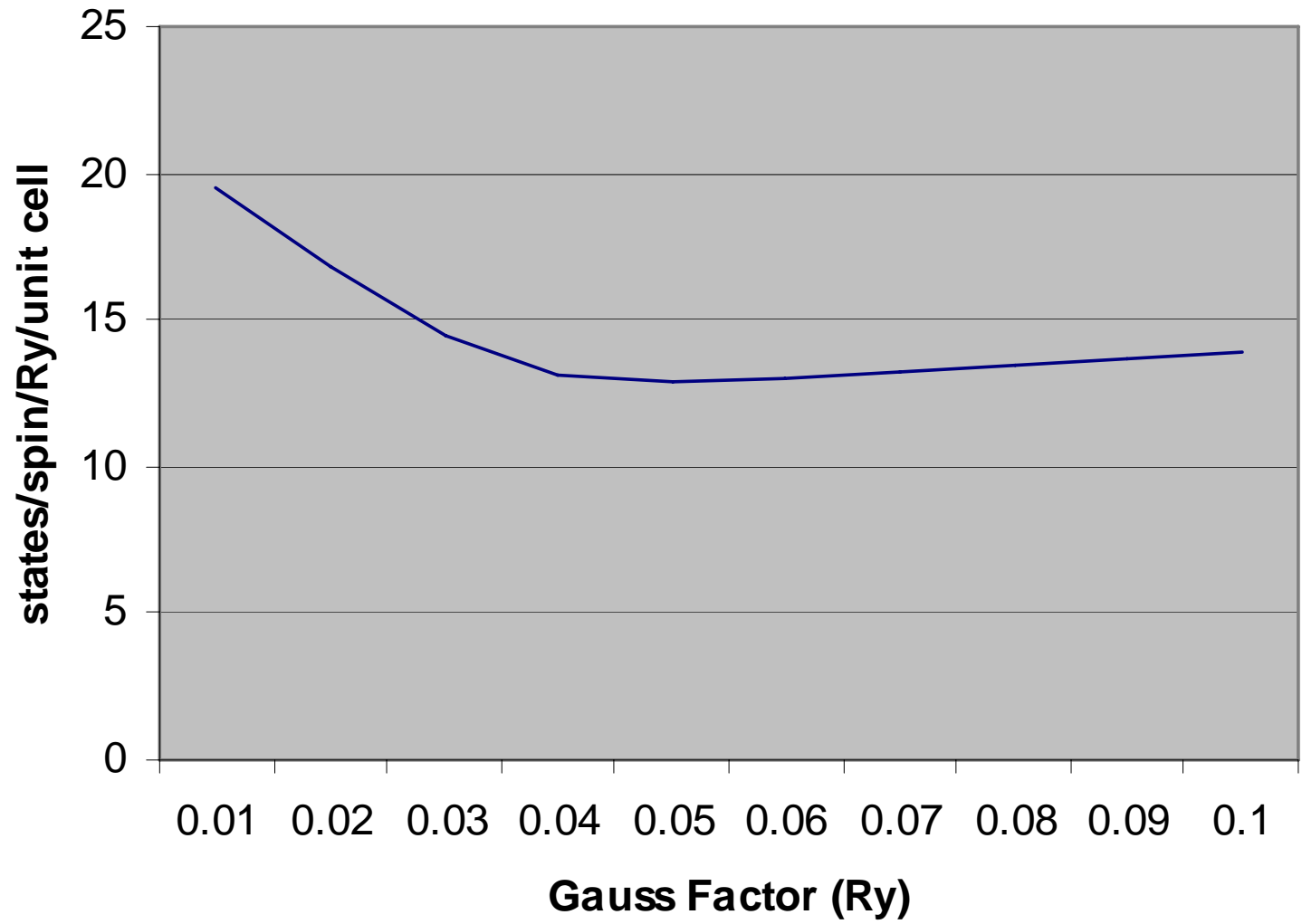


# Omega vs Representation

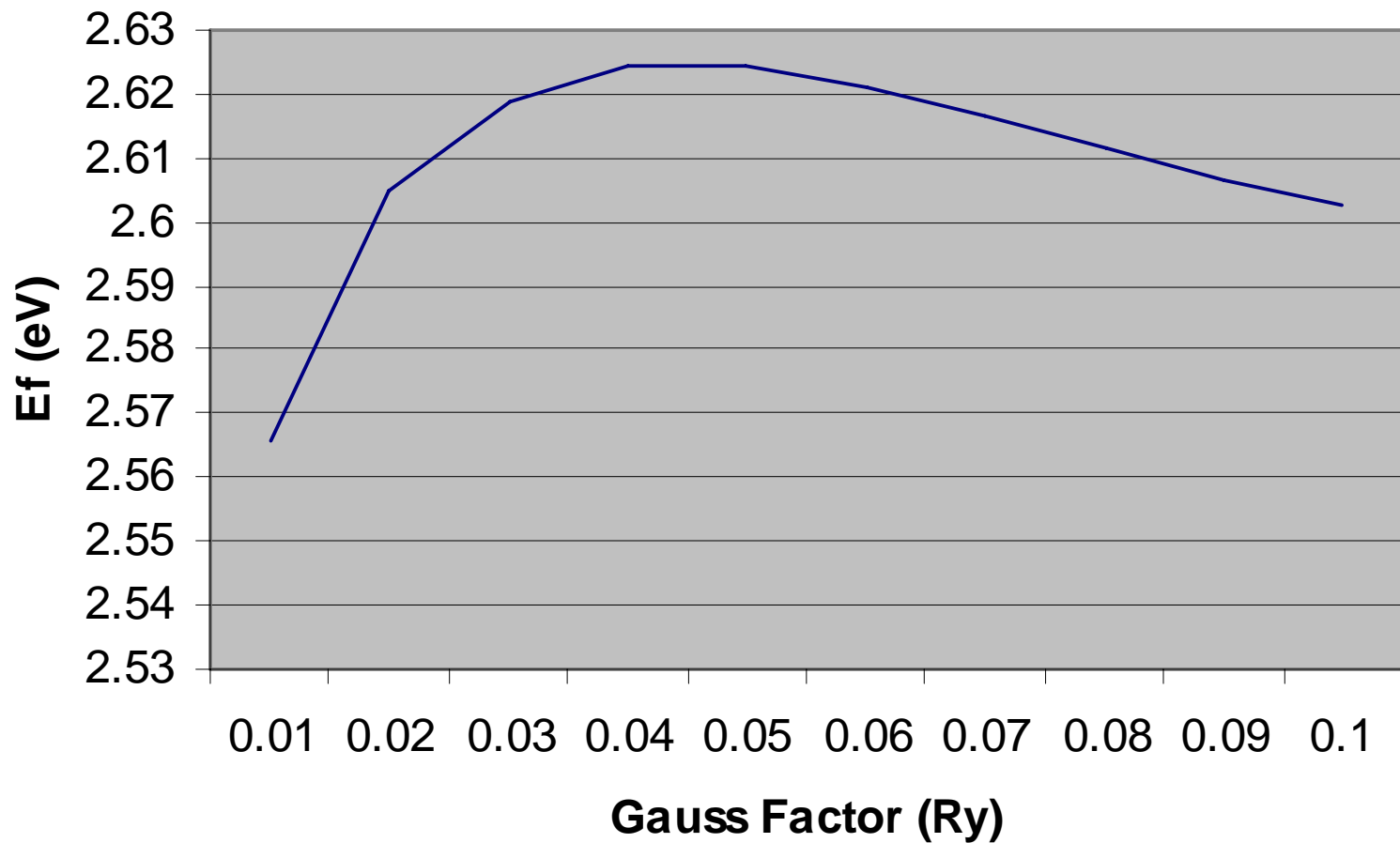


- B\_u 1
- A\_u 2
- A\_g 3
- B\_g 4
- B\_u 5
- B\_g 6
- A\_u 7
- A\_g 8
- A\_u 9
- A\_g 10
- B\_u 11
- B\_g 12
- B\_u 13
- B\_g 14
- A\_u 15
- A\_g 16
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- B\_g 18
- A\_u 19
- A\_u 20
- A\_g 21
- A\_g 22
- B\_u 23
- B\_g 24

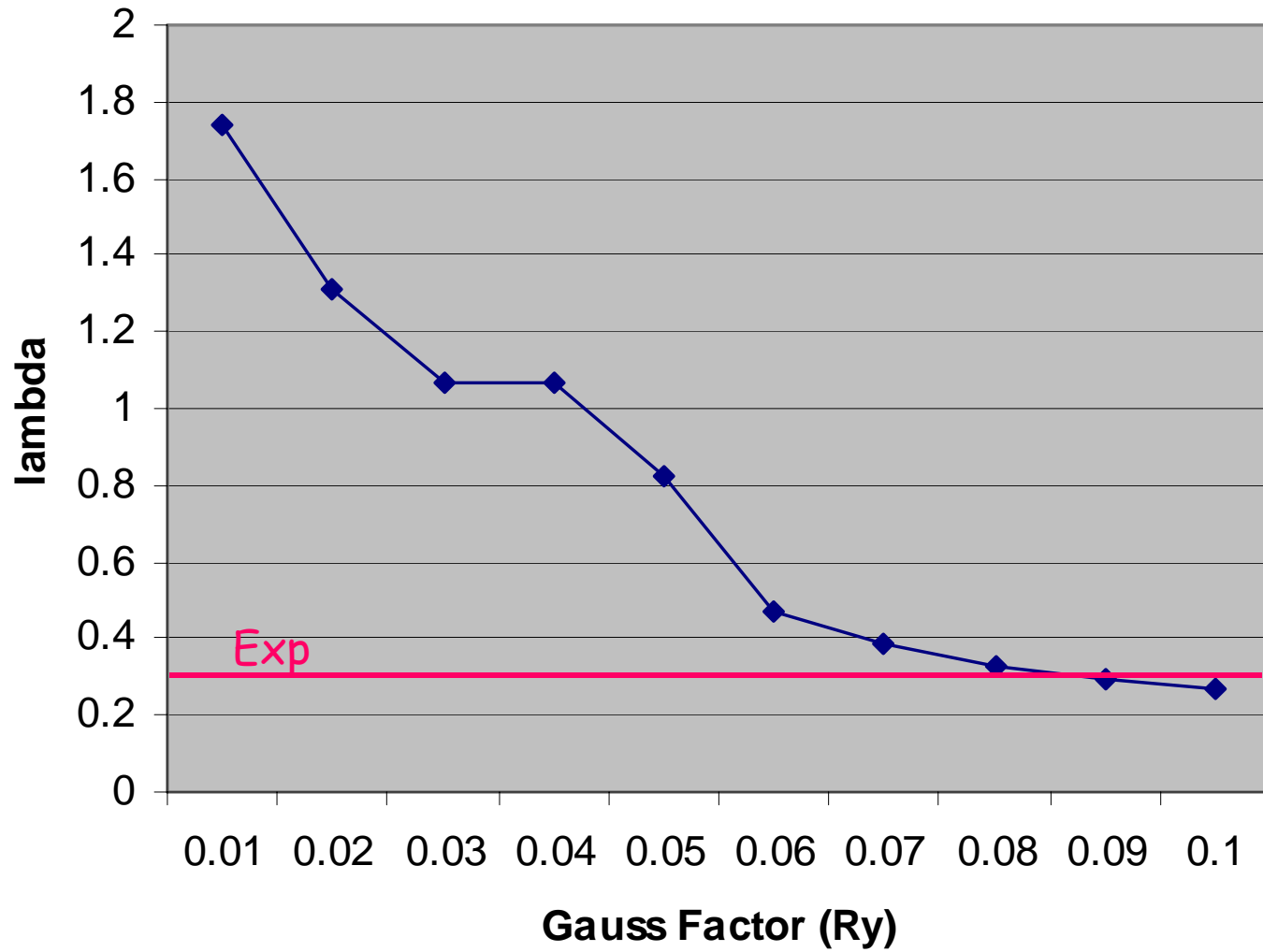
# DOS



### Fermi Energy



Total Lambda (q = 0,0,0 (Gamma))



# To-Do List

- Get access to some more flops (BlueGene?)
- Compute "nesting vectors"

$$X_q = \sum_k \delta(\epsilon_k - \epsilon_F) \delta(\epsilon_{k+q} - \epsilon_F)$$

- Compute Eliashberg and compare with Binnig tunneling
- Compute full lambda
- Dope (e.g., Br & ?)