

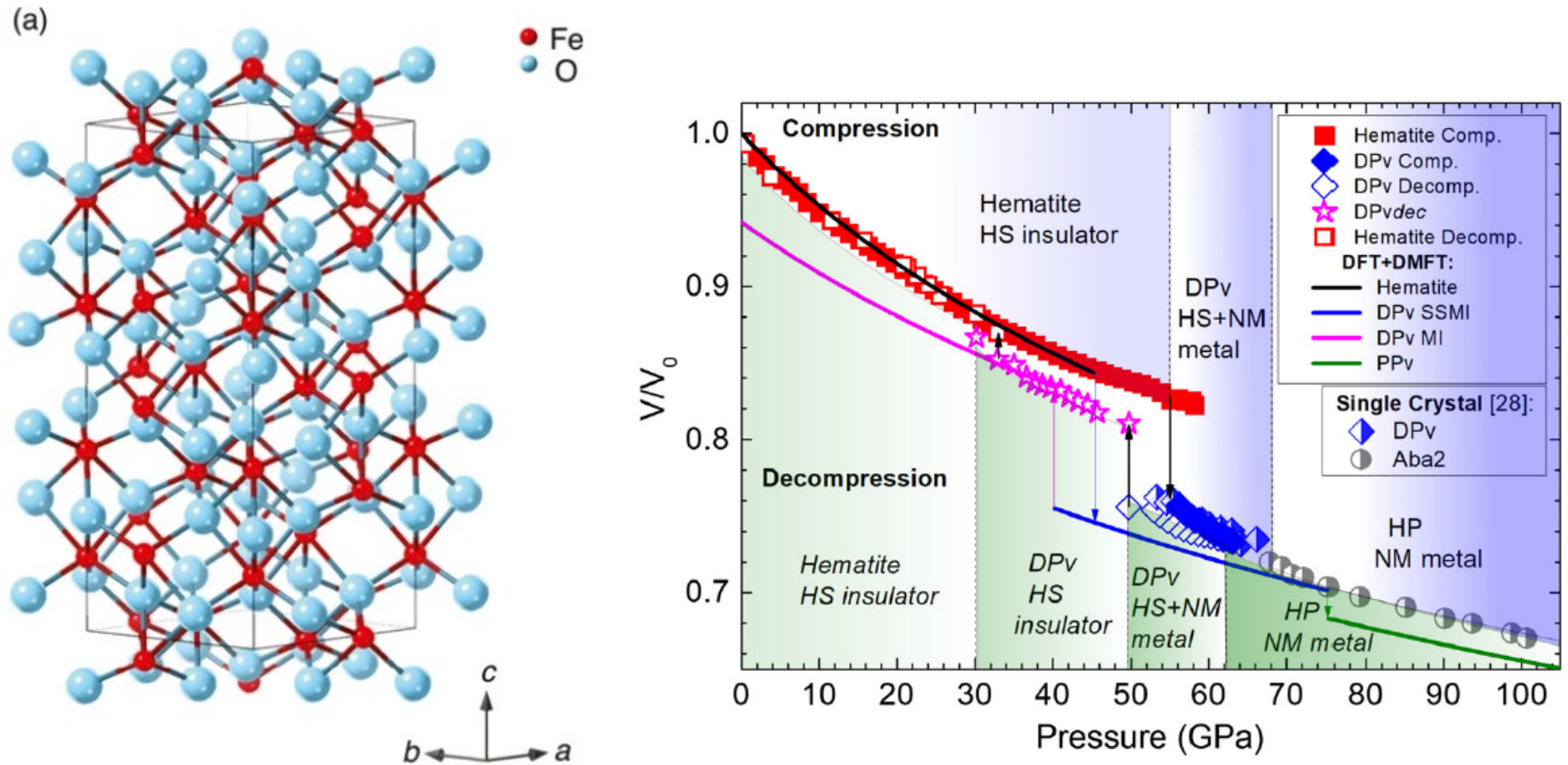


Things we can calculate and things we can not

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WISE-Wallenberg Initiative Materials Science

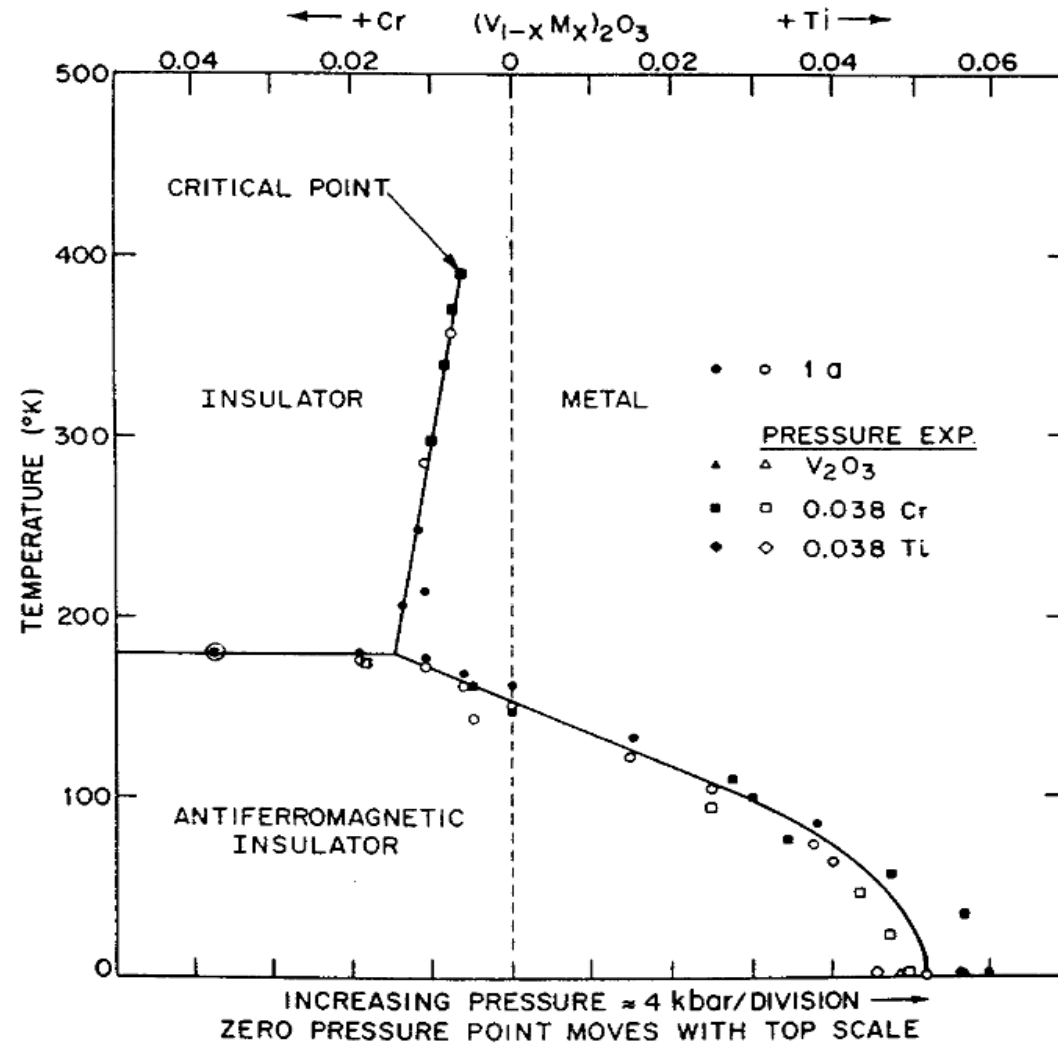


ESS (European Spallation Source) and Fe_2O_3

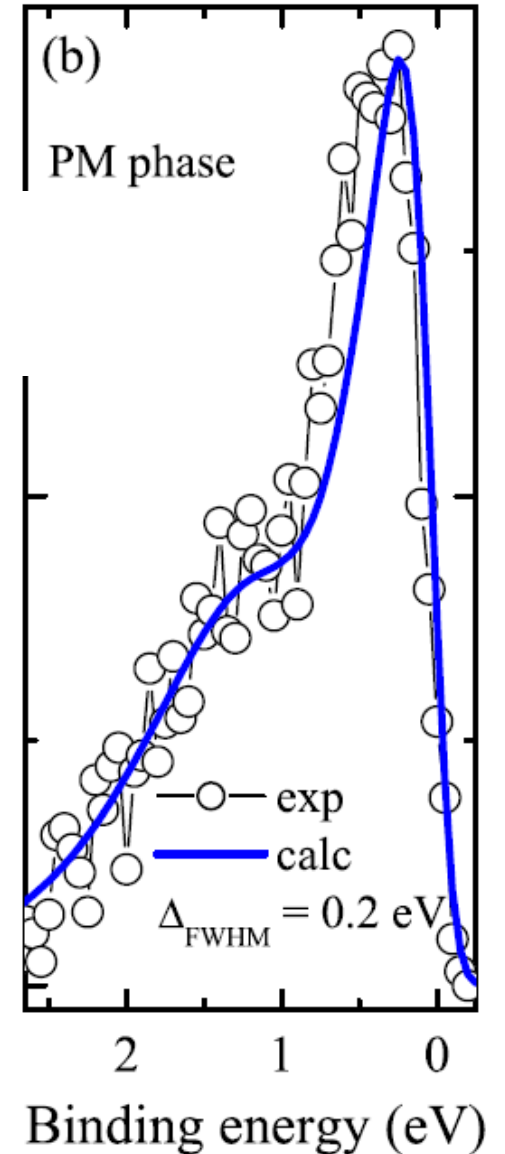




MAX IV, photoelectron spectroscopy

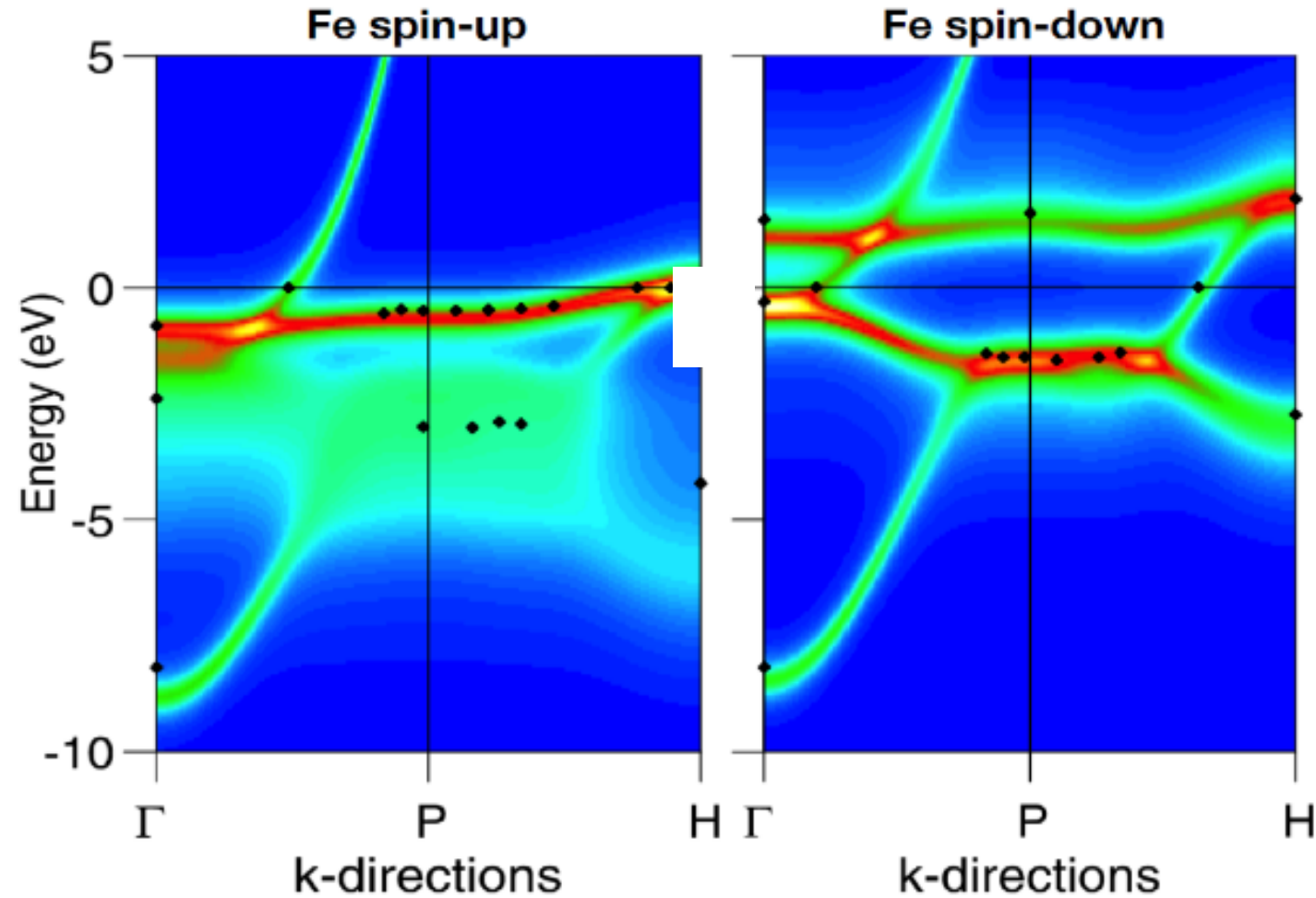


PRL 97, 116401 (2006)





MAX IV, Bloch beam line for ARPES



*Lichtenstein och Katsnelson,
J.Phys. Cond. Matt. **11**, 1037 (1999)*



MAX IV, Topological edge states

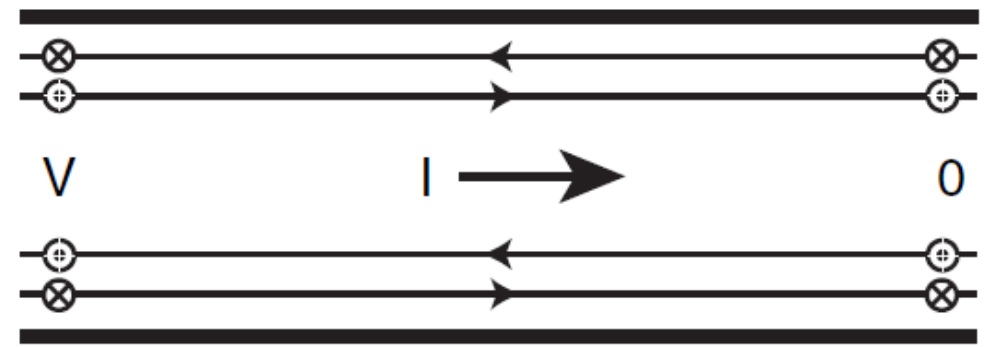
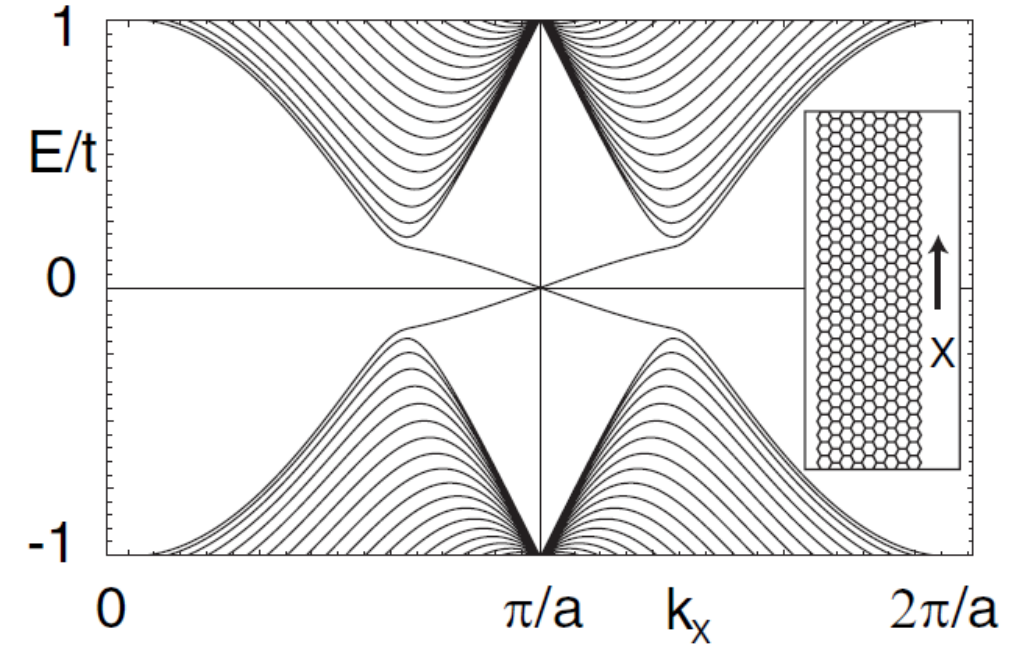
$$\sigma_{xy}^s = \frac{e}{2\pi}$$

$$\sigma_0^{xy} = \nu e^2 / (2\pi\hbar)$$

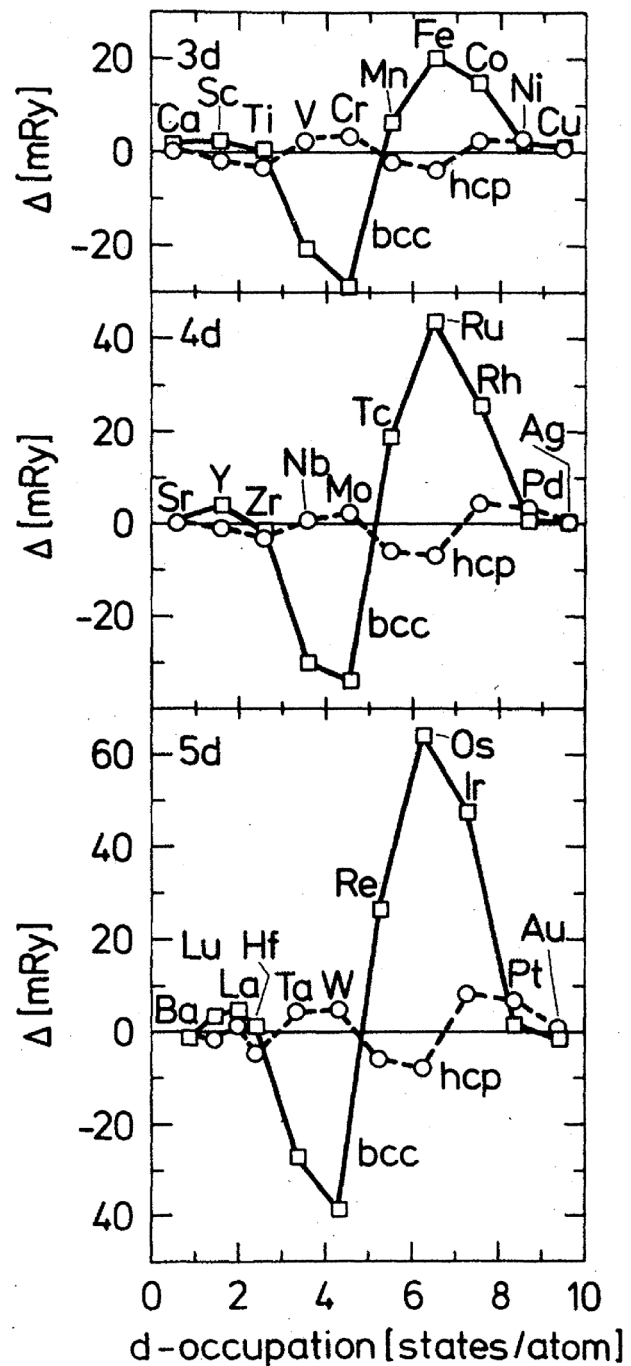
$$\nu_n(\mu) = \frac{1}{2\pi} \int d^2\mathbf{k} \mathcal{F}_n^{xy}(\mathbf{k}) P_{\text{BZ}}(\mathbf{k}) n_n(\mathbf{k}, \mu)$$

$$\mathcal{A}_n^a(\mathbf{k}) = -i \langle \psi_n(\mathbf{k}) | \nabla_{\mathbf{k}}^a \psi_n(\mathbf{k}) \rangle,$$

$$\mathcal{F}_n^{ab}(\mathbf{k}) = \nabla_{\mathbf{k}}^a \mathcal{A}_n^b(\mathbf{k}) - \nabla_{\mathbf{k}}^b \mathcal{A}_n^a(\mathbf{k})$$



Kane & Mele, Phys. Rev. Lett. 95, 226802 (2005)
 Haldane, Phys. Rev. Lett. 93, 206602 (2004)

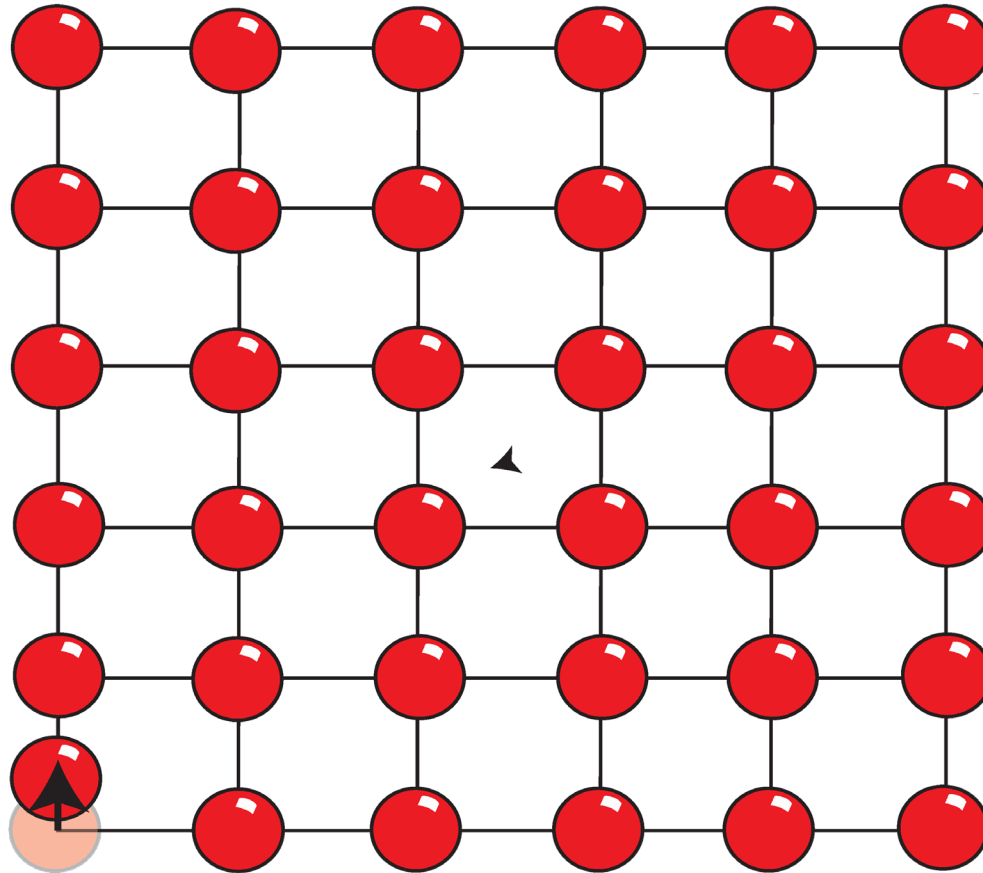


Crystal structures from DFT

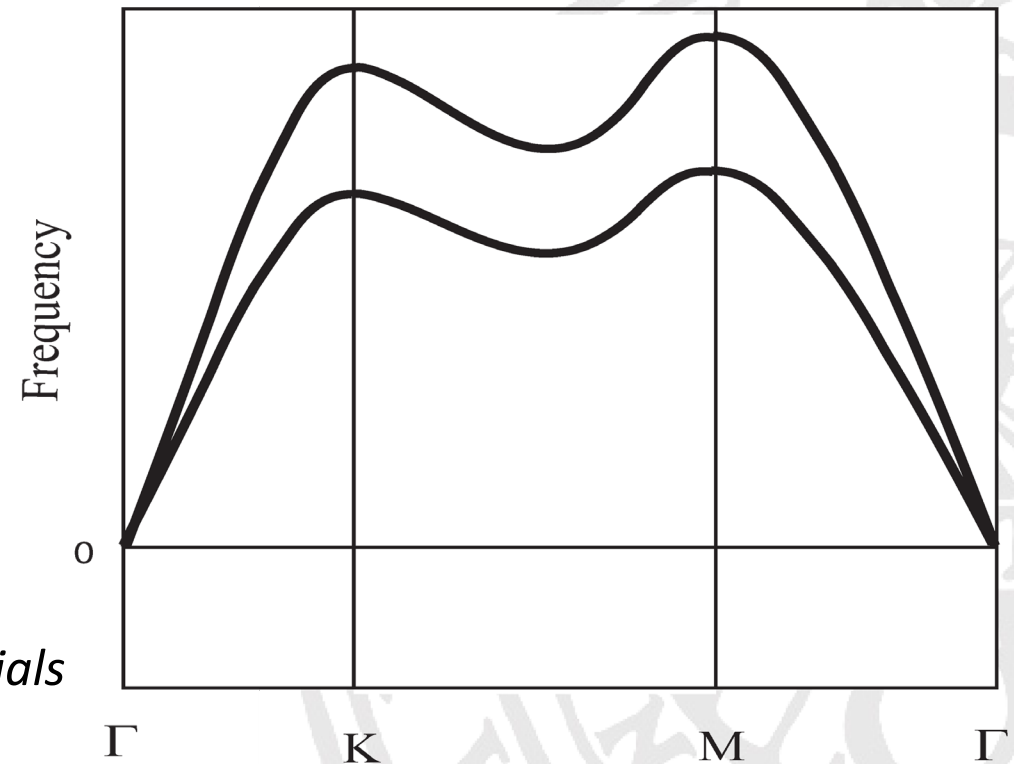
H.L.Skriver, Phys. Rev. B
31, 1909 (1985).



Lattice dynamics



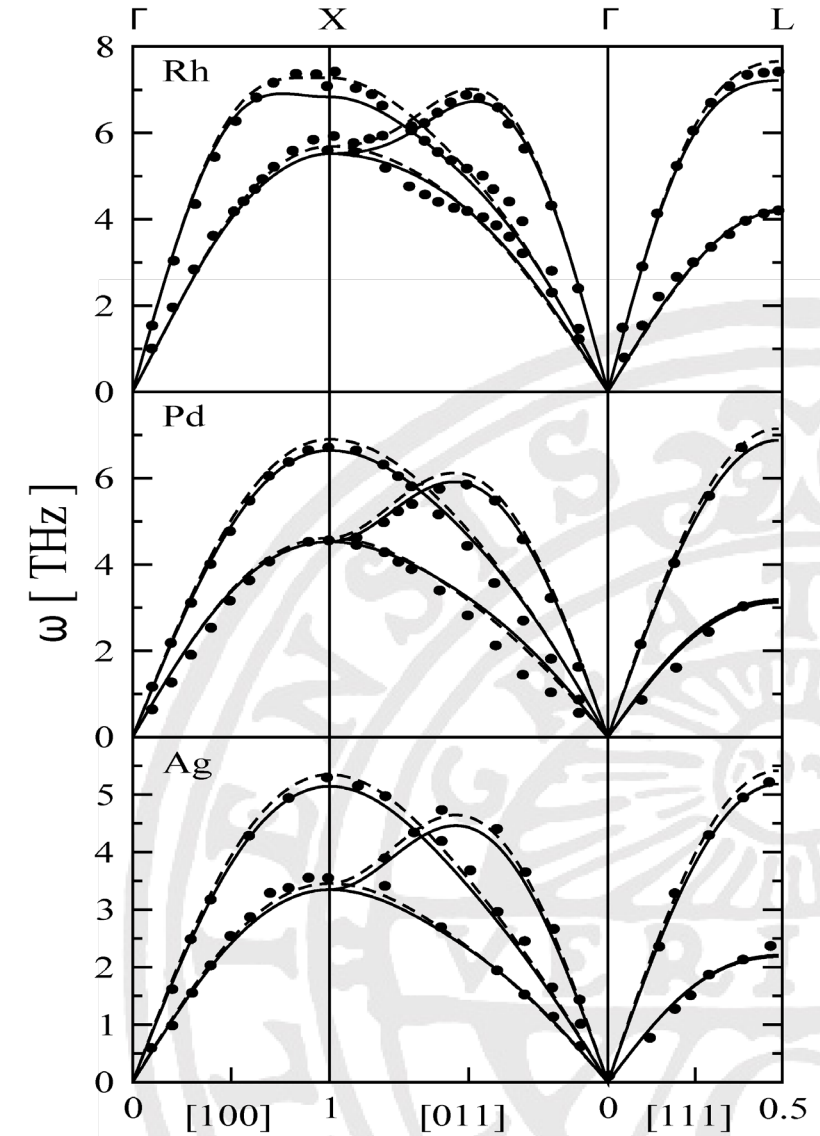
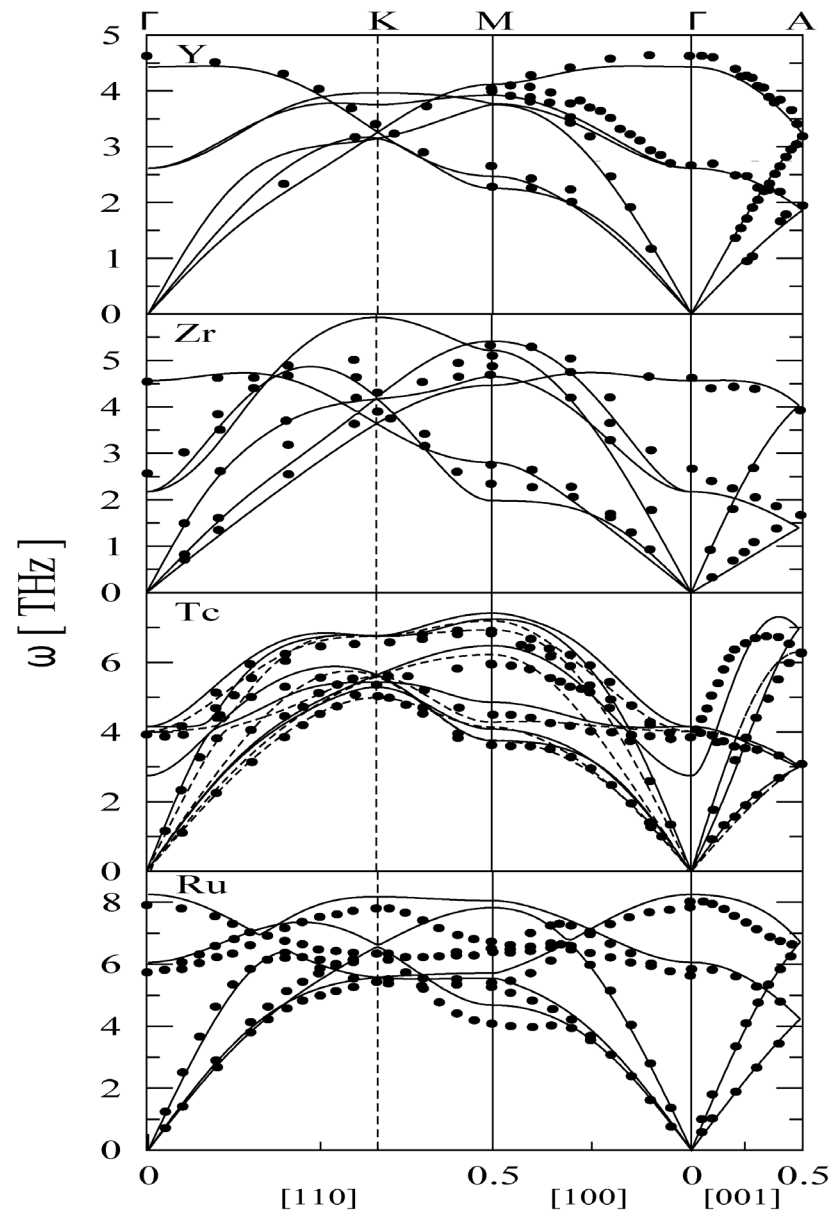
$$\mathbf{R} = \mathbf{R}_0 + \mathbf{U} \Rightarrow \bar{\bar{\Phi}}(\mathbf{R})$$
$$\Rightarrow \bar{\bar{D}}(\mathbf{k}) = \sum_{\mathbf{R}} \bar{\bar{\Phi}}(\mathbf{R}) e^{-i\mathbf{R}\mathbf{k}} \Rightarrow \omega_{\mathbf{k}s}^o$$



G.Grimvall, *Thermophysical properties of materials*
Elsevier 1999



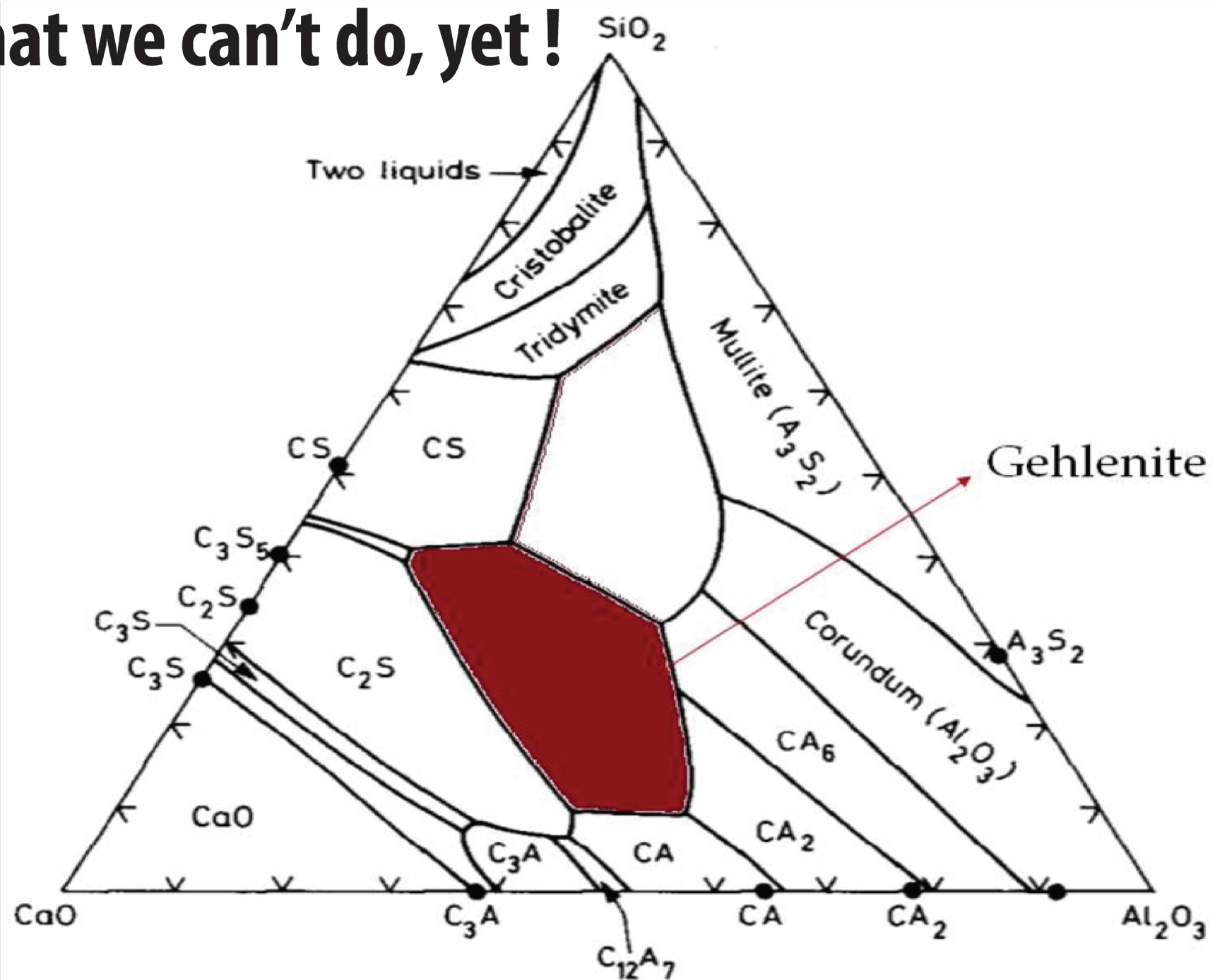
Phonons of selected transition metals



Souvatzis et al., PRB 77, 24110 (2008)

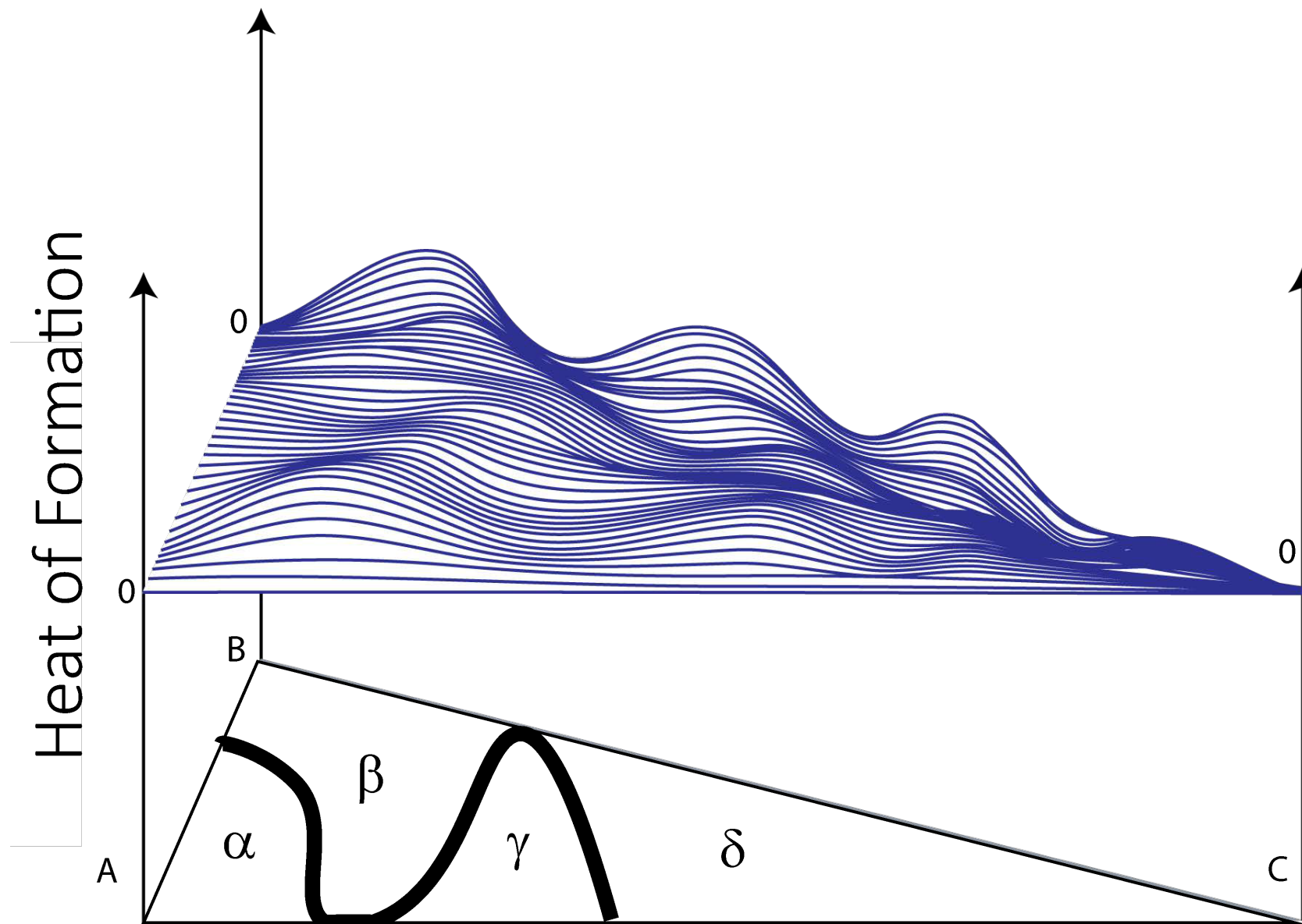


What we can't do, yet!





Error corrected DFT for accurate energies





Error corrected DFT for accurate energies

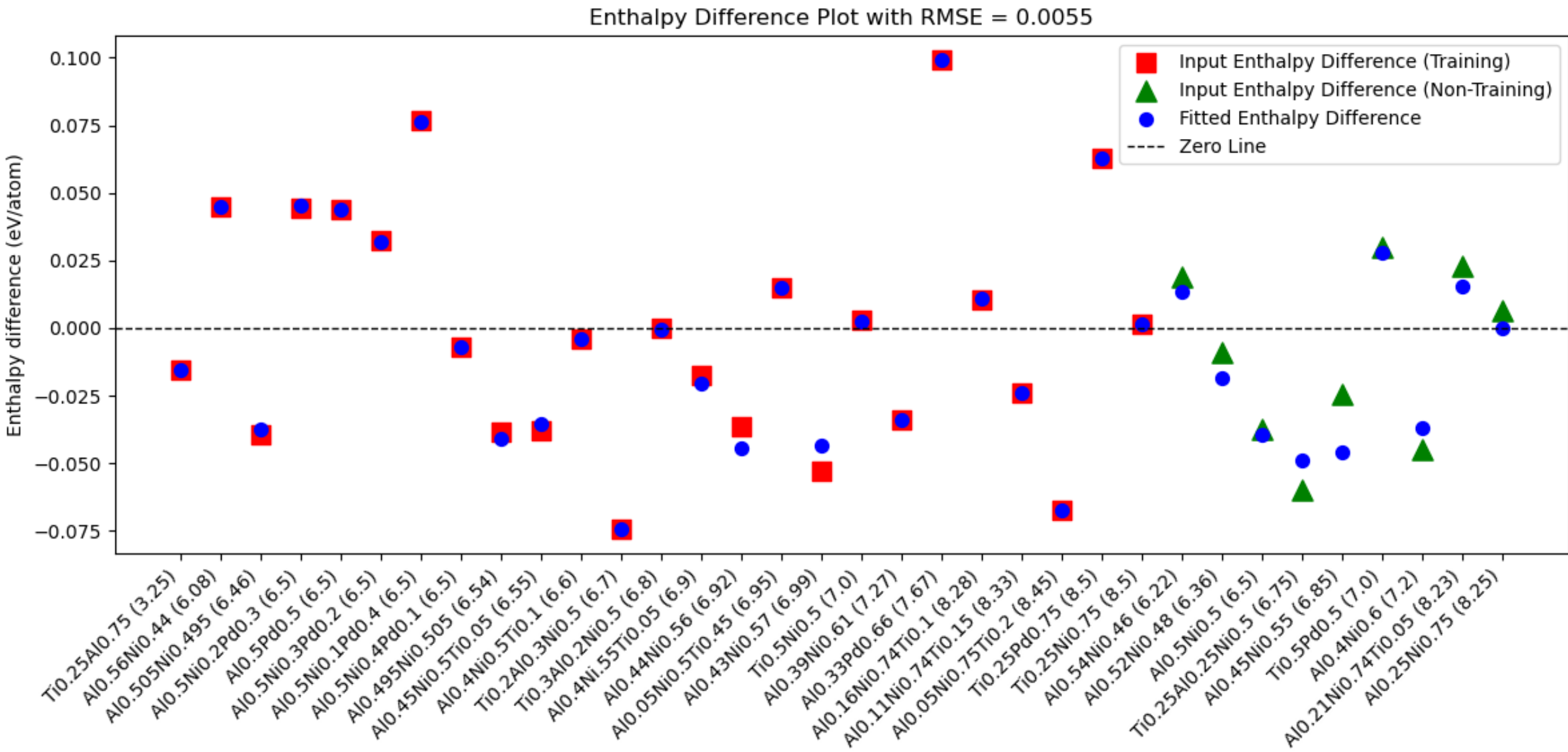
$$H_f(A_{x_A} B_{x_B} C_{x_C} \dots) = H(A_{x_A} B_{x_B} C_{x_C} \dots) - x_A H(A) - x_B H(B) - x_C H(C) - \dots$$

$$H_{\text{Corr}} = H_{\text{DFT}} - H_{\text{expt}}$$

$$H_{\text{corr}} = \mathbf{w}^T \mathbf{X} + b$$

X input parameters showing where in the phase diagram the system lies, **w** and **b** part of the ML network $\rightarrow H_{\text{Corr}}$ for any concentration

Comparing experimental and DFT-EC heats of formation





The density of materials

