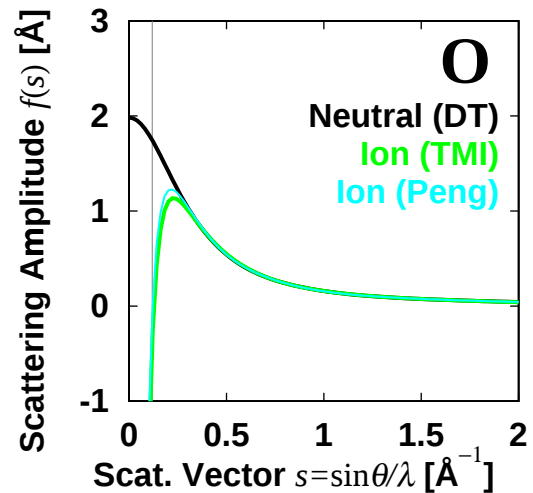
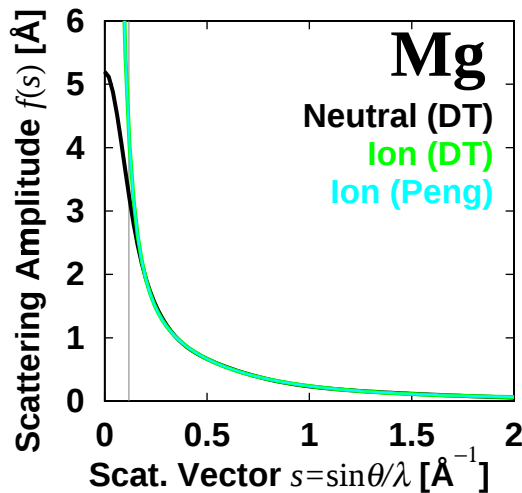


Fitting procedure for MgO

• Scattering factors

	Mg ²⁺	O ²⁻
Green	DT: Doyle and Turner, <i>Acta Cryst.</i> A24 (1968) 390	TMI: Tanji, Masaoka and Ito, <i>J. Elec. Microsc.</i> 38 (1989) 409
Blue	Peng: Peng, <i>Acta Cryst.</i> A54 (1998) 481	



• Temperature factors

$$B_{\text{Mg}} = 0.305 \text{ \AA}^2, B_{\text{O}} = 0.340 \text{ \AA}^2 \quad \left(\text{Zuo, O'Keeffe, Rez and Spence, } \textit{Phys. Rev. Lett.} \text{ } \mathbf{78} \text{ (1997) 4777} \right)$$

• Fitting parameters

- γ : Absorption coefficient ($\gamma = 0, 1, \dots, 10 \%$)
- x : Ionicity ($x = 0, 5, 10, \dots, 100 \%$)

$$\text{Scattering factor, } f, \text{ is given by } f = x f_{\text{ion}} + (1 - x) f_{\text{neu}}$$

