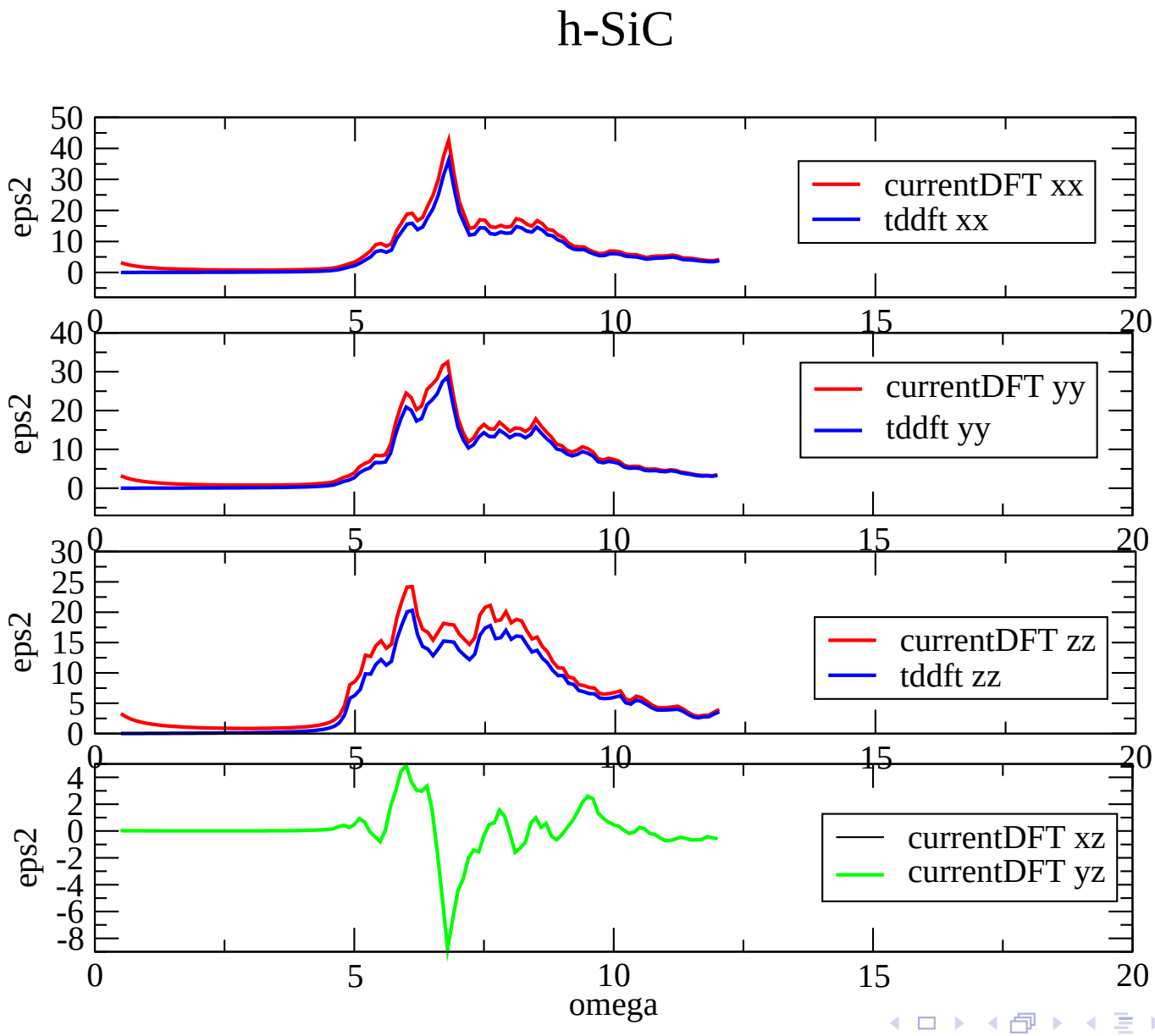
Transverse Modes in Optics and EELS

Hannes Hübener, Ralf Hambach

30. 01. 2009

Optics ($q \longrightarrow 0$)

TDCDFT: Optics



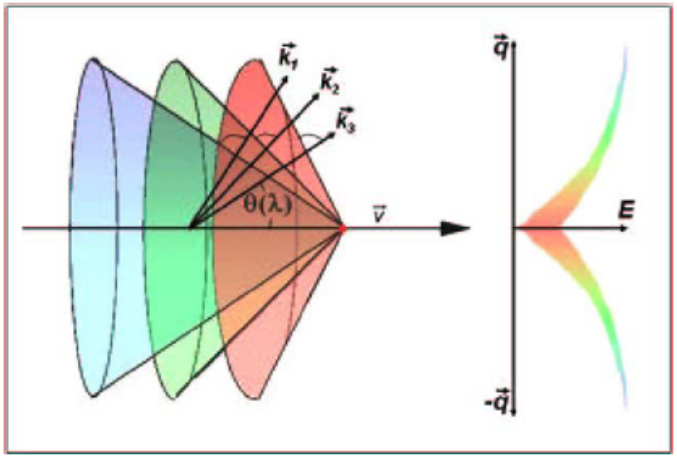
EELS ($q > 0$)

What is Cerenkov Radiation ?

(a) electron (v) faster than light (c/n):

$$\cos^2\alpha = \frac{c^2}{\Re\epsilon v^2} = \frac{1}{\Re\epsilon\beta^2}$$

Cerenkov condition: $\Re\epsilon\beta^2 > 1$



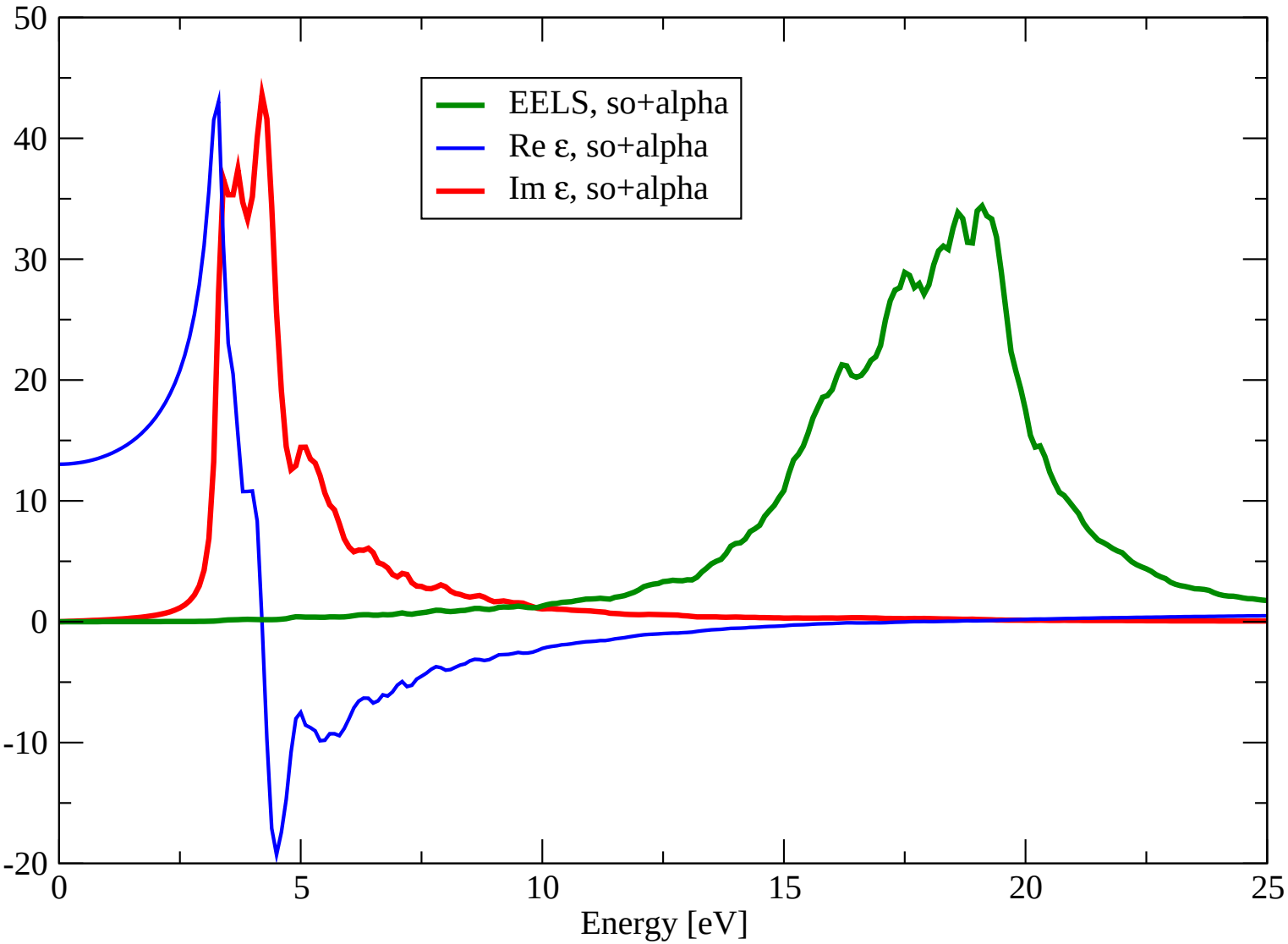
[Stöger-Pollach *et al.*, Micron **37**, 396 (2006)]

(b) Köger formula (ϵ of homogeneous media, E^e transverse):

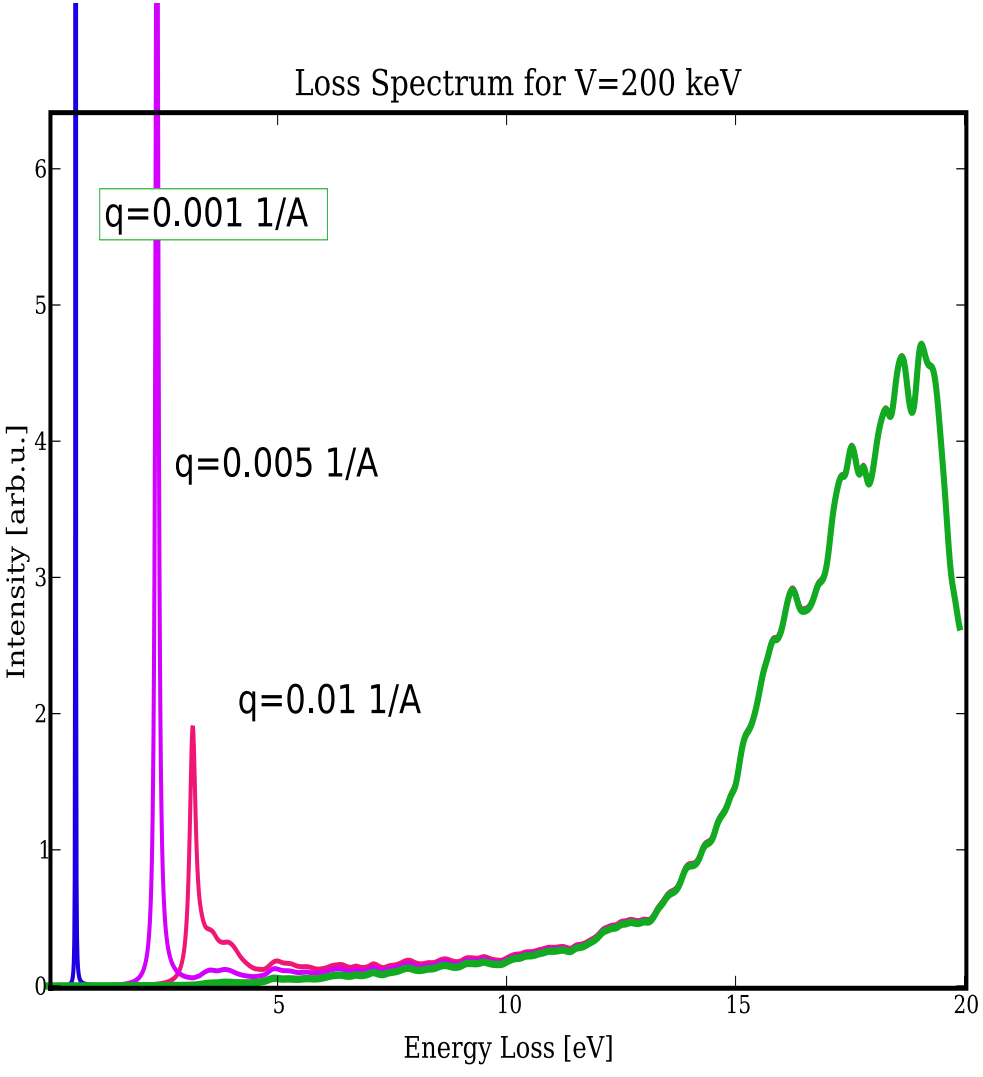
$$\frac{\partial P_V(\omega, q_\perp)}{\partial\omega\partial^2 q_\perp} = -\frac{De^2}{\pi^2\hbar v^2}\frac{1}{q^2}\Im\left[\frac{1}{\epsilon_L(\omega)} - \frac{\beta^2 q_\perp^2}{q^2 - (\frac{\omega}{c})^2\epsilon_L(\omega)}\right]$$

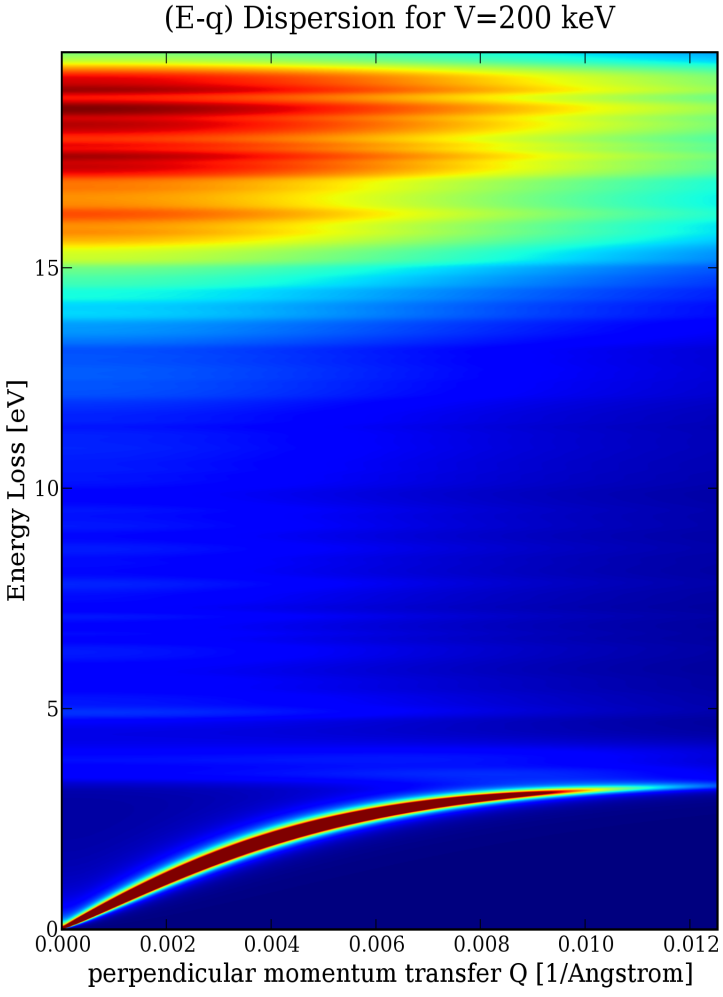
[E. Kröger, Zeitschrift für Physik A Hadrons and Nuclei **216**, 115 (1968)]

Silicon: unretarded

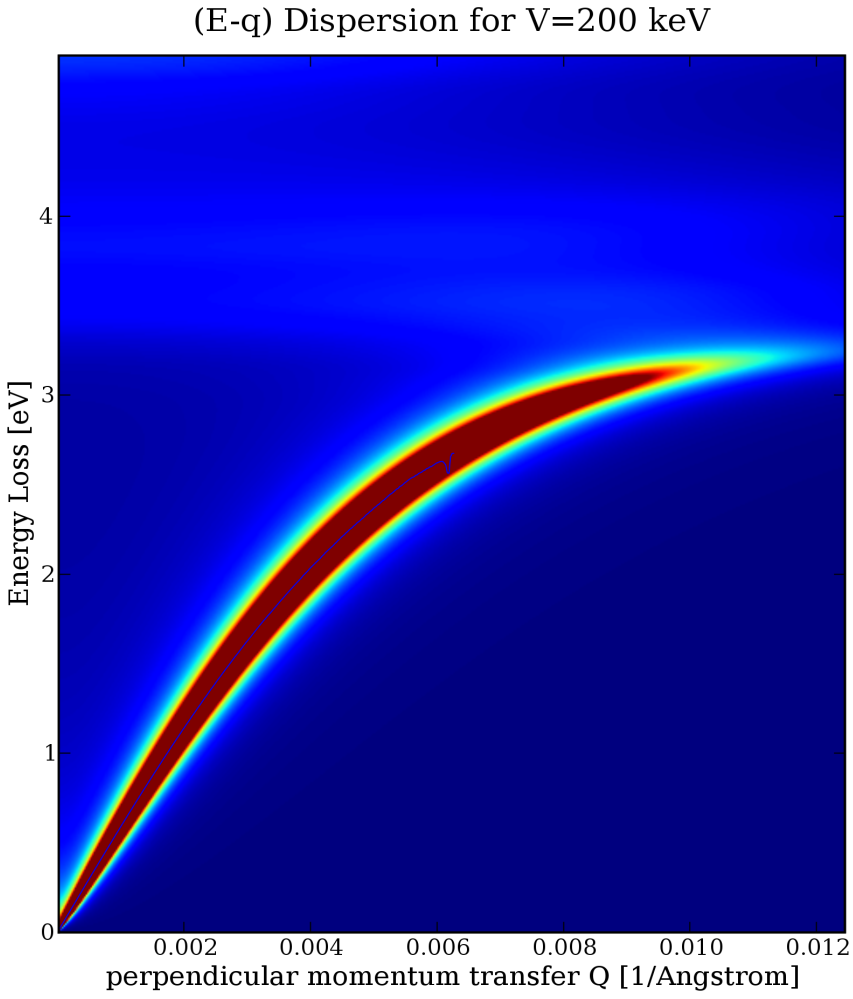


Silicon: retarded (200 keV)





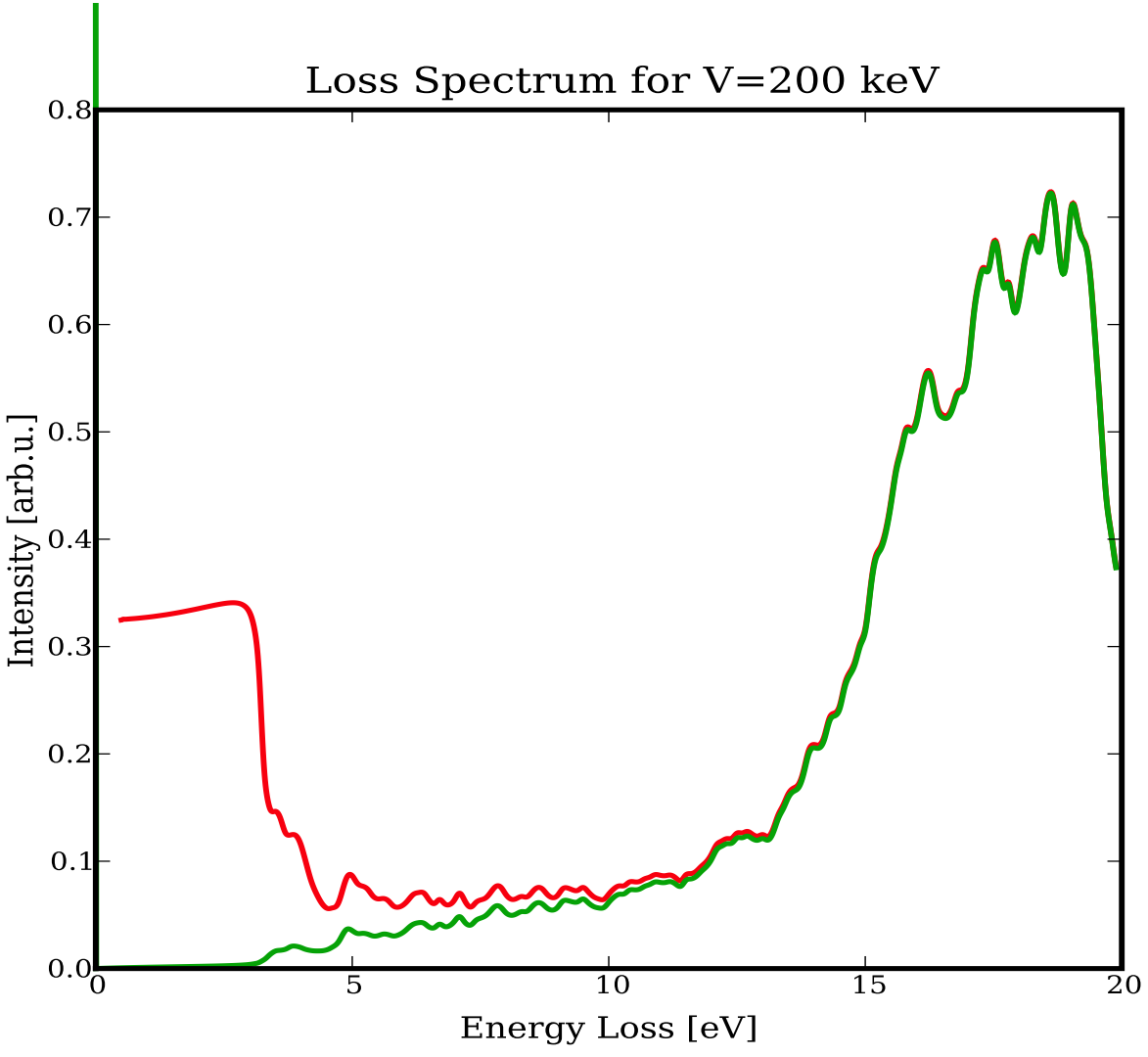
Silicon: retarded (200 keV)



- acceleration:
  $E_0 = 200\mathrm{keV}$, $\beta = 0.7$
- photon energy:
  $E < 5\mathrm{eV}$, $q_{||} < 0.004\text{Å}^{-1}$
- photon momentum:
  $\theta < 0.04\mathrm{mrad}$, $q_{\perp} < 0.01\text{Å}^{-1}$
- very sharp ω-q dispersion:

$$\omega^2(q) = \frac{c^2 q_{\perp}^2}{\Re\epsilon(\omega) - 1/\beta^2}$$

Silicon: retarded (200 keV)



- finite q-resolution:
  $\theta_{\text{max}} = 0.05\text{mrad}$,
  $q_{\perp}^{\text{max}} = 0.013\text{Å}^{-1}$
- integration:
  $$\int_0^{q_{\perp}^{\text{max}}} dq_{\perp} q_{\perp} S(q_{\perp}, \omega)$$

Transverse Waves in ϵ ?

- longitudinal Dyson equation (RPA) for $\epsilon_{LL}^{-1} = 1 + v\chi_{LL}$:

$$\chi_{LL} = \chi^0_{\rho\rho} + \chi^0_{\rho\rho}\, v\, \chi_{LL}$$

- full Dyson equation for tensors $\chi = \chi^{\alpha\beta}_{\boldsymbol{GG'}} = \left(\begin{smallmatrix} \chi_{LL} & \chi_{LT} \\ \chi_{TL} & \chi_{TT} \end{smallmatrix}\right)$:

$$\chi = \chi^0_{jj} - \chi^0_{jj}\, \mathcal{O}^{-1}\, \chi, \qquad \mathcal{O} = \nabla \times (\nabla \times \cdot) - \partial_t^2$$

- optics for $q > 0$ (beyond dipole approximation)
- LFE in optics (mixing of T and L ?)
- LFE in EELS (beyond Köger)
- other applications of CDFT