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No class on Wednesday, November 09, 2016

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Homework Assignment #06: Chapter 6: 1,6,7,8,9 due Monday, November 14, 2016

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Homework Assignment #06: Chapter 6: 1,6,7,8,9 due Monday, November 14, 2016

Homework Assignment #7: Chapter 7: 2,3,9,10,11 due Monday, November 28, 2018

Synthesis of Sn-graphite nanocomposites



XRD shows a small amount of Sn metal in addition to $Sn_3O_2(OH)_2$





In situ battery box



Pouch cell clamped against front window in helium environment

C. Segre (IIT)

PHYS 570 - Fall 2016

In situ battery box



Suitable for both transmission and fluorescence measurements

C. Segre (IIT)

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Fresh electrode can be fit with $Sn_3O_2(OH)_2$ structure which is dominated by the near neighbor Sn-O distances



Fresh electrode can be fit with $Sn_3O_2(OH)_2$ structure which is dominated by the near neighbor Sn-O distances

Only a small amount of metallic Sn-Sn distances can be seen

C. Segre (IIT)



Reduction of number of Sn-O near neighbors and 3 Sn-Li paths characteristic of the $\rm Li_{22}Sn_5$ structure



Metallic Sn-Sn distances appear but Sn-Li paths are still present, further reduction in Sn-O near neighbors.





Number of Li near neighbors oscillates with the charge/discharge cycles but never returns to zero



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In situ cell promotes accelerated aging because of Sn swelling and the reduced pressure of the thin PEEK pouch cell assembly



C. Pelliccione, E.V. Timofeeva, and C.U. Segre, "In situ XAS study of the capacity fading mechanism in hybrid $Sn_3O_2(OH)_2$ /graphite battery anode nanomaterials" *Chem. Mater.* **27**, 574-580 (2015).

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The dispersion relation of electrons in a solid, $\mathcal{E}(\vec{q})$ can be probed by angle resolved photoemission

$$\begin{aligned} \mathcal{E}_{kin}, \ \theta & \longrightarrow \ \mathcal{E}(\vec{q}) \\ \mathcal{E}_{kin} &= \frac{\hbar^2 q_v^2}{2m} = \hbar \omega - \phi - \mathcal{E}_B \\ \mathcal{E}_B &= \mathcal{E}_F - \mathcal{E}_i \end{aligned}$$



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Electrons with lower energy will fall inside this circular path while those with higher enegy will fall outside



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assuming a solution of the form

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The amplitude of the response has a resonance and dissipation

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The radiated (scattered) electric field at a distance R from the electron is directly proportional to the electron's acceleration with a retarded time t' = t - R/c (allowing for the travel time to the detector).

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$$\begin{split} f_s &= \frac{\omega^2 + \left(-\omega_s^2 + i\omega\Gamma\right) - \left(-\omega_s^2 + i\omega\Gamma\right)}{\left(\omega^2 - \omega_s^2 + i\omega\Gamma\right)} \\ &= 1 + \frac{\omega_s^2 - i\omega\Gamma}{\left(\omega^2 - \omega_s^2 + i\omega\Gamma\right)} \\ &\approx 1 + \frac{\omega_s^2}{\left(\omega^2 - \omega_s^2 + i\omega\Gamma\right)} \end{split}$$

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the second term being the dispersion correction

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Single oscillator dispersion terms

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$$f_{s}^{\prime} = \frac{\omega_{s}^{2}(\omega^{2} + \omega_{s}^{2})}{(\omega^{2} - \omega_{s}^{2})^{2} + (\omega\Gamma)^{2}}$$

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$$\sigma_T = \left(\frac{8\pi}{3}\right) \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2} r_0^2$$

this shows a frequency dependence with a peak at $\omega\approx\omega_{s}$

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PHYS 570 - Fall 2016

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for an electron bound to an atom, we can now generalize

this shows a frequency dependence with a peak at $\omega\approx\omega_{s}$

if $\omega \ll \omega_{s}$ and when $\Gamma \rightarrow$ 0, the cross-section becomes

$$\sigma_{free} = \left(\frac{8\pi}{3}\right) r_0^2$$

$$\sigma_T = \left(\frac{8\pi}{3}\right) \frac{\omega^4}{(\omega^2 - \omega_s^2)^2 + (\omega\Gamma)^2} r_0^2$$



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The total cross-section for scattering from a free electron is

for an electron bound to an atom, we can now generalize

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when $\omega \gg \omega_s$, $\sigma_T \rightarrow \sigma_{free}$

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Refractive index

$$n^{2} = 1 + \left(\frac{e^{2}\rho}{\epsilon_{0}m}\right)\frac{1}{\left(\omega_{s}^{2} - \omega^{2} - i\omega\Gamma\right)}$$

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C. Segre (IIT)

Refractive index

$$\begin{split} n^2 &= 1 + \left(\frac{e^2\rho}{\epsilon_0 m}\right) \frac{1}{(\omega_s^2 - \omega^2 - i\omega\Gamma)} \\ &= 1 + \left(\frac{e^2\rho}{\epsilon_0 m}\right) \frac{\omega_s^2 - \omega^2}{(\omega_s^2 - \omega^2)^2 + (\omega\Gamma)^2} + i \frac{\omega\Gamma}{(\omega_s^2 - \omega^2)^2 + (\omega\Gamma)^2} \end{split}$$



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