Optical properties of bulk Te and Te nanowires

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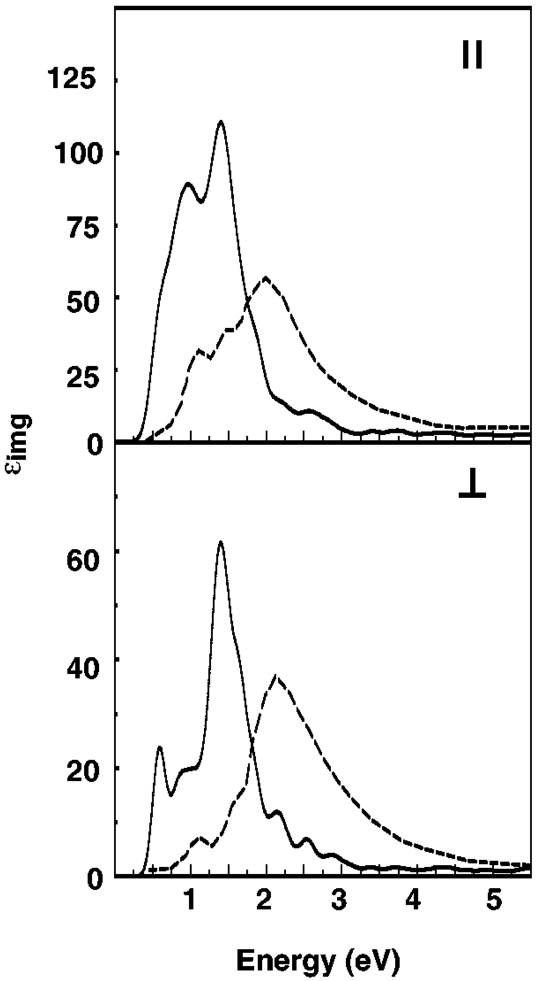
Basics about Te

- What is Te (Telurium)?
  - Semiconductor
  - 6th group family
  - Used in alloys for data storage
  - Used as element in the photovoltaic panels

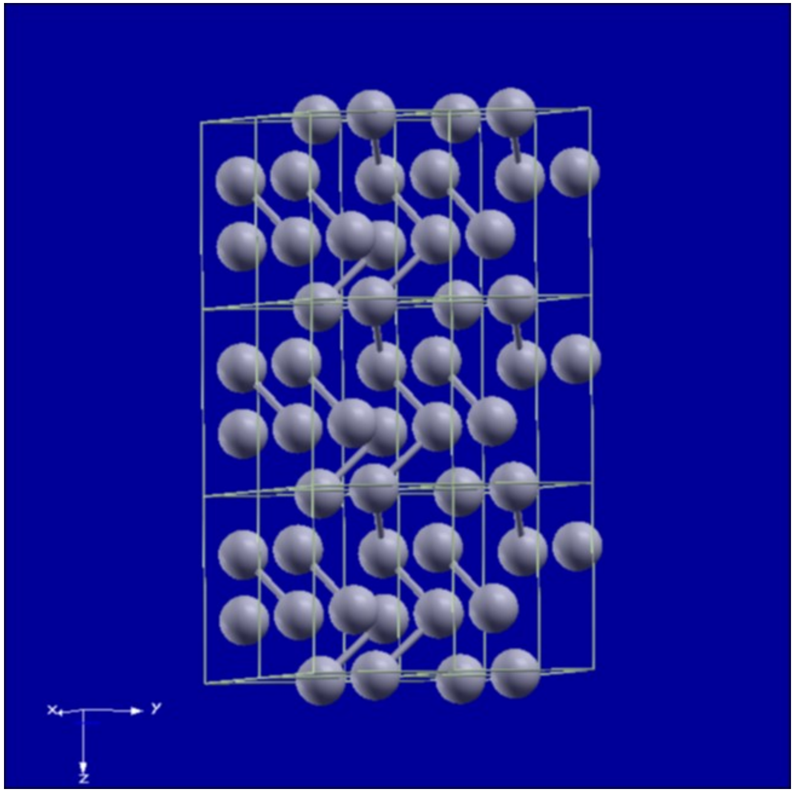
Motivation

- Why study Te ?
  - Study optical properties of bulk and nanowires
  - Previous study without local fields (physical review B 75,245437)



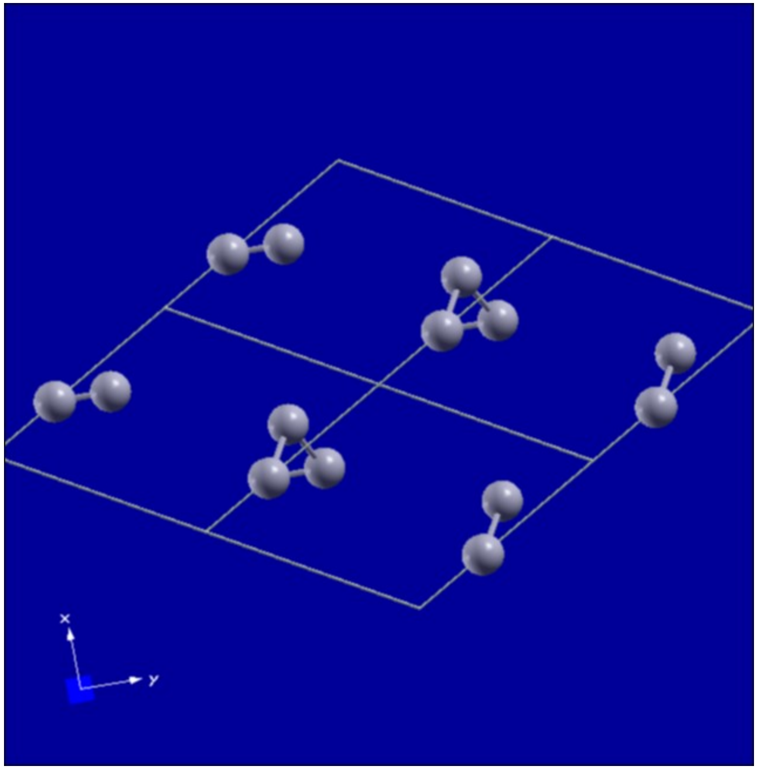
Bulk structure

- Hexagonal structure
- Composed by wires in helix chains

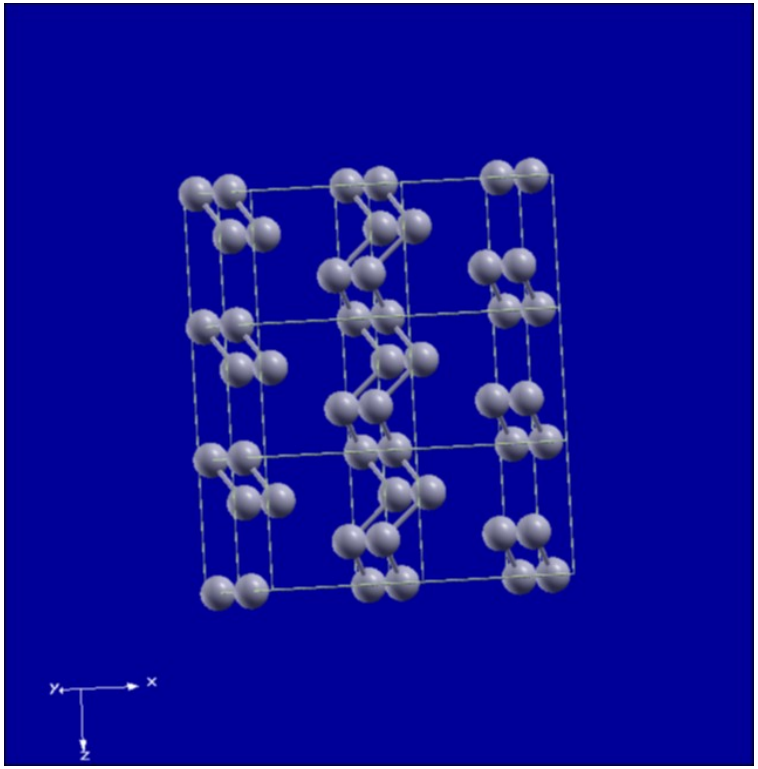


Nanowire structure

x-y-plane



z-direction



Applied theories

- DFT Formulas
  - Used with ABINIT

Khon-Sham equation :

$$\rho(\mathbf{r}) = \sum_{i=1}^{N} |\phi_i(\mathbf{r})|^2$$

$$E[\rho(\mathbf{r})] = T[\rho(\mathbf{r})] + \frac{1}{2}\int d\mathbf{r}d\mathbf{r}'\frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \int d\mathbf{r}v(\mathbf{r})\rho(\mathbf{r}) + E_{xc}[\rho(\mathbf{r})]$$

$$\left\{-\frac{1}{2}\nabla^2 + v(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} + \frac{\delta E_{xc}\rho(\mathbf{r})}{\delta\rho(\mathbf{r})}\right\}\phi_i(\mathbf{r}) = \varepsilon_i\phi_i(\mathbf{r})$$

Applied Theories

- RPA Approximation
  - Used with DP
    - Ground state calculation
    - Independent-Particle polarizability
    - Full po $\chi_0(\mathbf{r}, \mathbf{r}', \omega) = \sum_{v,c} \frac{(f_v - f_c)\phi_v^*(\mathbf{r})\phi_c(\mathbf{r})\phi_c^*(\mathbf{r}')\phi_v(\mathbf{r}')}{}$

$$\chi = \chi_0 + \chi_0(v + f_{xc})\chi,$$

Applied Theories

- RPA Approximation
  - Random Phase Approximation (RPA)

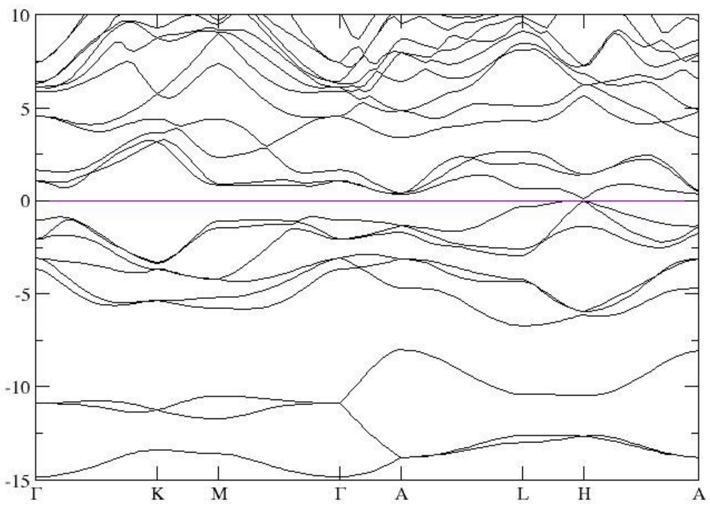
$$f_{xc} = 0$$

  - Dielectric function

$$\varepsilon^{-1} = 1 + v\chi$$

Results for the ground state

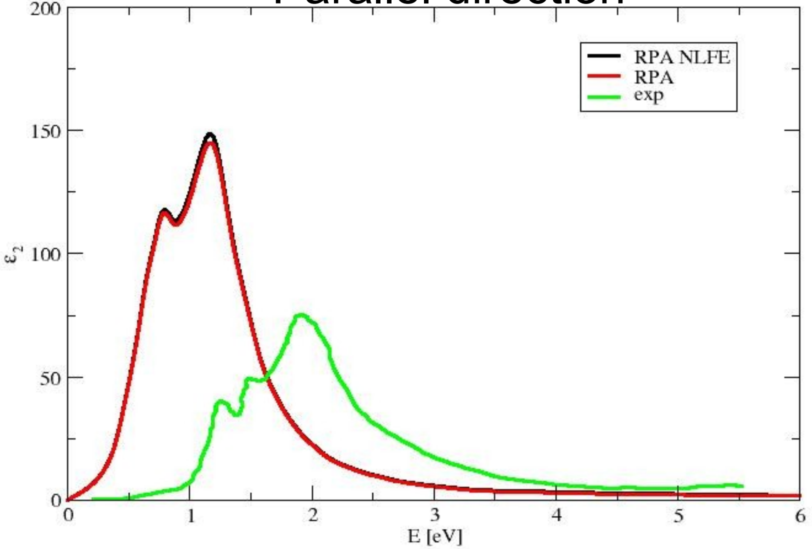
	ΩV	c/a	Gap
PBE Previous Study	33.95	1.33	0.150
PBE My Work	34.10	1.30	0.140 (with GGA Approximation)
Experimental	33.74	1.33	0.336



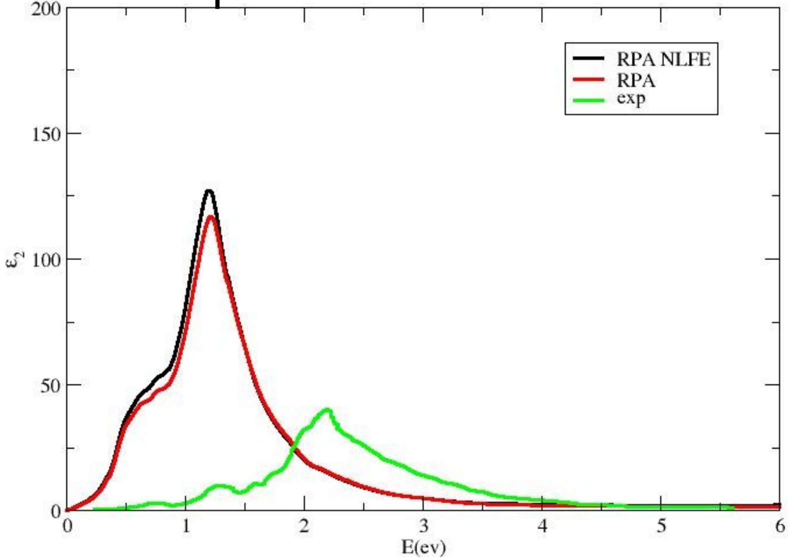
s and p levels separated

Bulk spectra

Parallel direction



Perpendicular direction



Local fields do not change spectra significantly

Nanowires spectra

- Futures studies for spectra :
  - Helix Te
  - Shell Te (with 21 atoms)
  - Double shell (with 57 atoms)
- Comparison with Bulk spectra

Conclusion

- Result not yet conclusive
- The local fields do not improve the spectra
- Calculations will be applied to the nanowires

Questions & Answers