Optics Beamline

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European Theoretical Spectroscopy Facility (ETSF)

22 October 2010

Outline

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Optics beamline

Coordinator: Dr. Olivia Pulci (`Olivia.Pulci@roma2.infn.it`)
University of Rome Tor Vergata, Rome, Italy

Phenomena: Linear optics (absorption spectra, cross sections, reflectance anisotropy, surface differential reflectivity, birefringence, chirality). Second Harmonic Generation.

Systems: Surfaces, dots, wires, nanotubes, molecules. Bulk materials. Amorphous materials. Liquids.

Theoretical methods: Density Functional Theory (DFT), Time-Dependent DFT (TDDFT). Many-body methods: GW approximation, Bethe-Salpeter equation (BSE). Tight binding, etc.

Nodes involved: All nodes. In particular Paris, San Sebastián, Rome, Jena, Modena.

Outline

Theories and Approximations

Linear Optical Absorption ($\sim$ 95%)

$$\text{Absorption} = \text{Im}\left\{\varepsilon_M\right\}$$

and related (birefringence, surface analysis: reflectance anisotropy, surface differential reflectivity).

Non-linear Optics ($\sim$ 5%)

$$\delta n = \chi \delta V_{ext} + \chi^{(2)} V_{ext} V_{ext} + \chi^{(3)} V_{ext} V_{ext} V_{ext} + ..$$

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Linear Optical Absorption

IPA - rough and very fast

$$Abs = \mathrm{Im}\chi^0_M \;\Rightarrow\; \chi^0 = \sum_{vc} \frac{\psi_v(\mathbf{r})\psi^*_c(\mathbf{r}')\psi_c(\mathbf{r})\psi^*_v(\mathbf{r}')}{\omega - (\epsilon_c - \epsilon_v) + i\eta}$$

relies only on a ground-state calculation.

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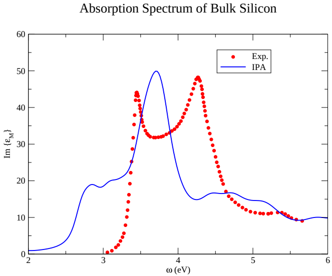

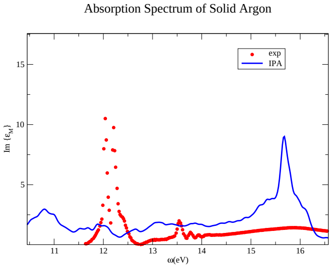

Linear Optical Absorption

TDDFT - standard and fast

$$Abs = \mathrm{Im}\varepsilon_M \quad \Rightarrow \quad \varepsilon^{-1} = 1 + v\chi$$

$$\chi = \chi^0 + \chi^0(v + f_{xc})\chi$$

- ✗ Essentially (today) within LDA or GGA...
- √ ... but heavy development for better functionals.

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GW+BSE - state-of-the-art and cumbersome

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- √ Good results
- × Cumbersome calculations

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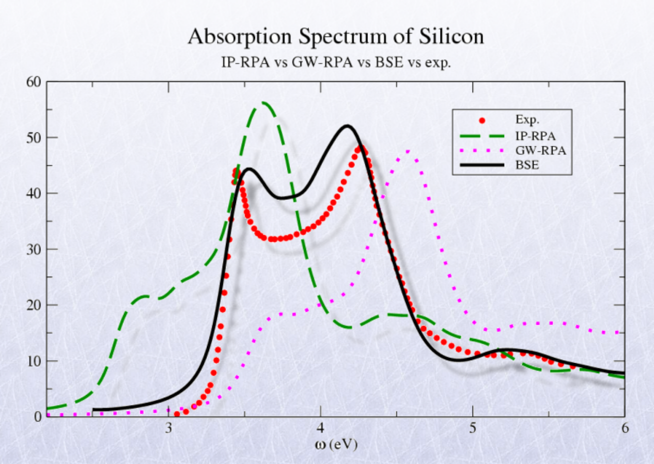
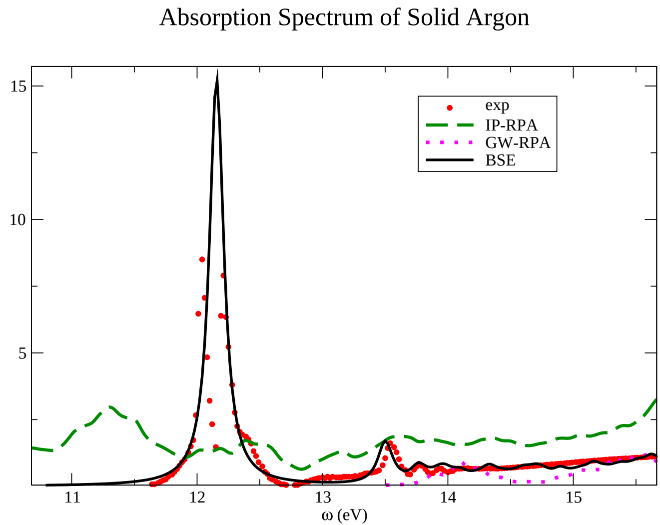
Optical Absorption



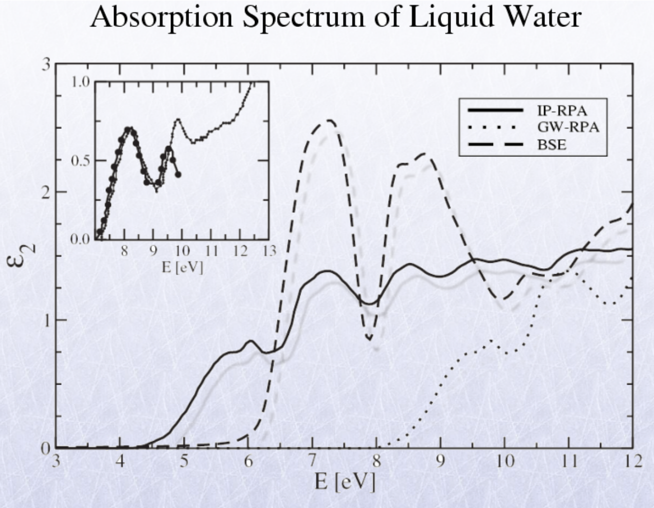
Albrecht *et al.* PRL **80**, 4510 (1998)

Optical Absorption



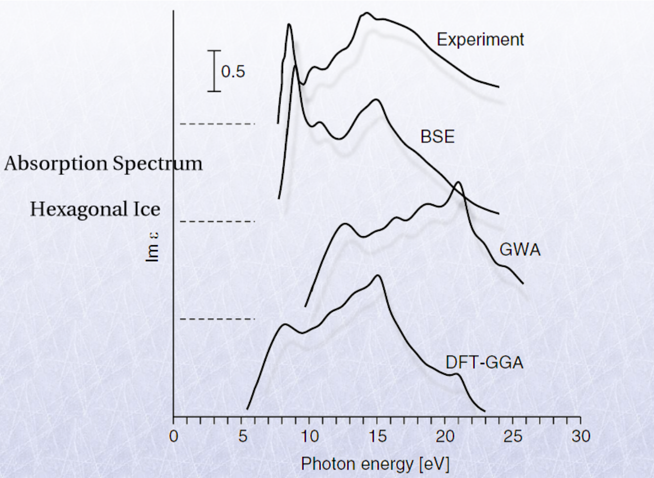
F.Sottile *et al.* PRB **76**, 161103 (2007)

Optical Absorption



Garbuio *et al.*, PRL **97**, 137402 (2006)

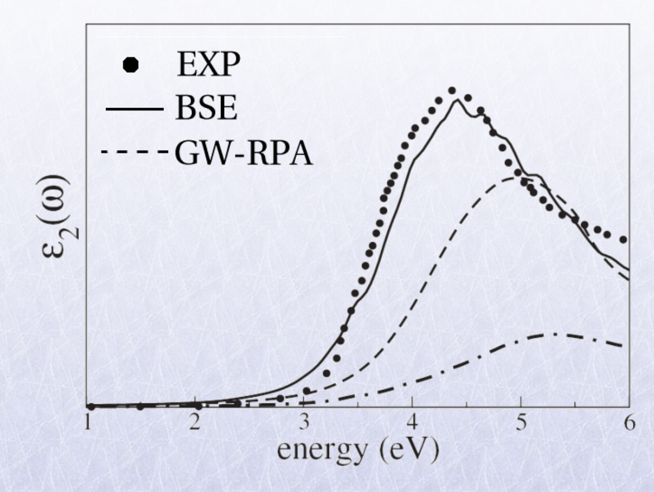
Optical Absorption



Hahn *et al.*, PRL **94**, 37404 (2005)

Optical Absorption

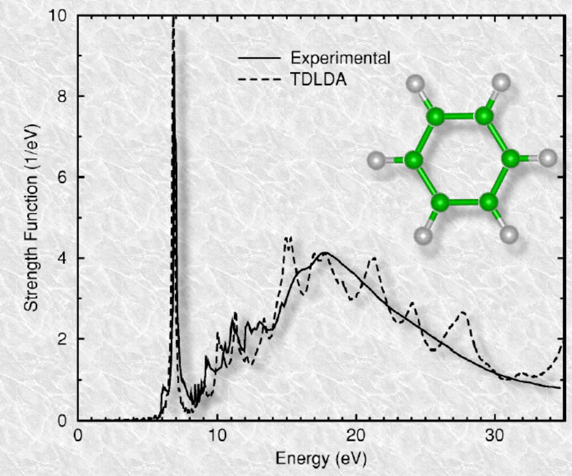
Silicon Nanowire



Bruno *et al.*, PRL **98**, 036807 (2007)

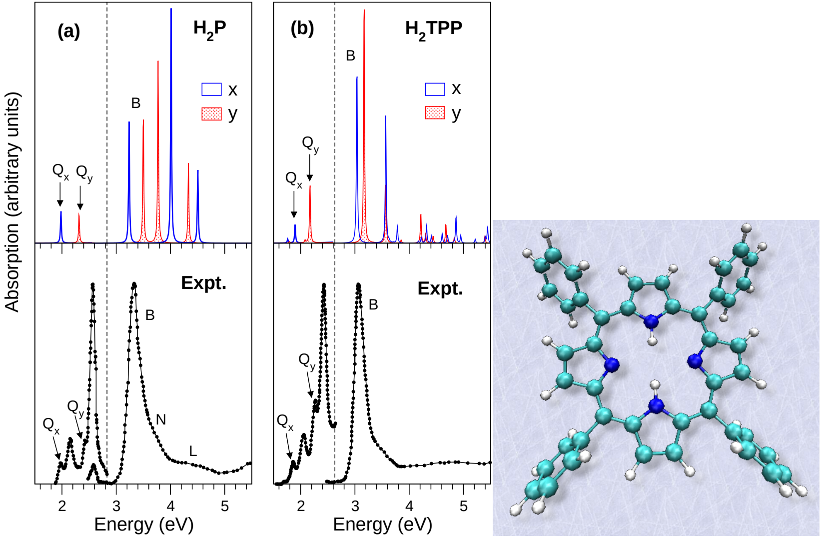
Optical Absorption

Benzene - TDLDA!



Bertsch *et al.*, J. Chem Phys. **115**, 4051 (2001)

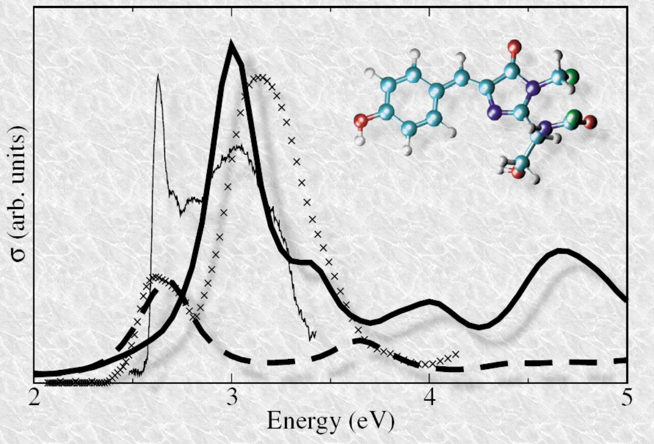
Biomolecules: simulation as a powerful analysis tool



Palummo *et al.*, J. Chem. Phys. **131**, 084102 (2009)

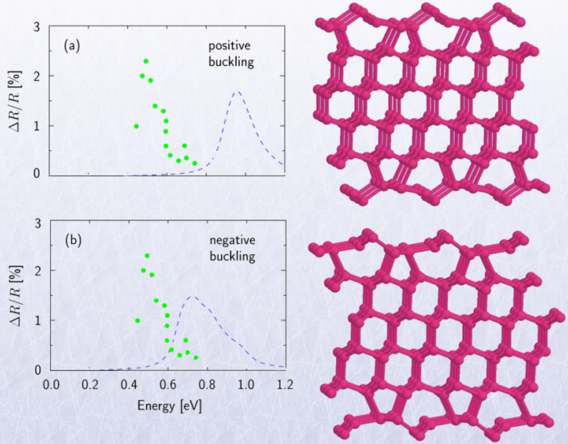
Biomolecules: simulation as a powerful analysis tool

Analysis - Green Fluorescent Protein



M.Marques *et al.* Phys.Rev.Lett **90**, 258101 (2003)

Surface Analysis - SDR of Ge(111)(2x1)



Rohlfing *et al.*, PRL **85**, 005440 (2000)

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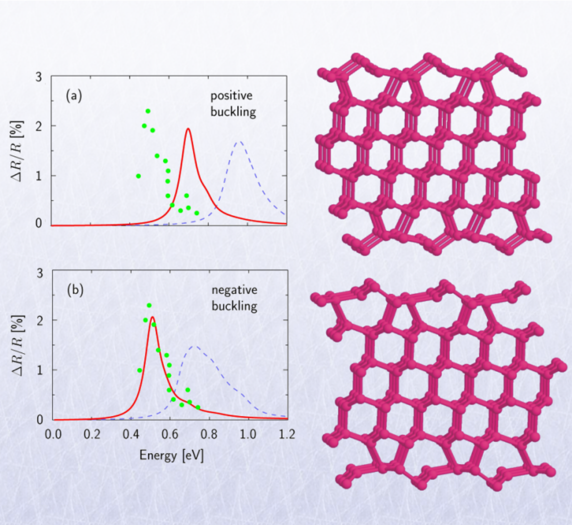
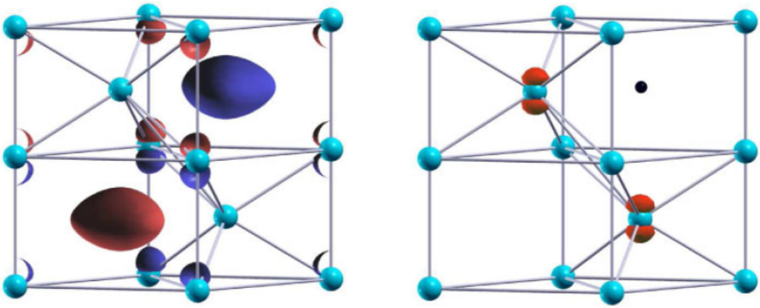


Rohlfing *et al.*, PRL **85**, 005440 (2000)

Sodium under pressure: how to look at an exciton



M.Gatti et al, Physical Review Letter **104**, 216404 (2010).

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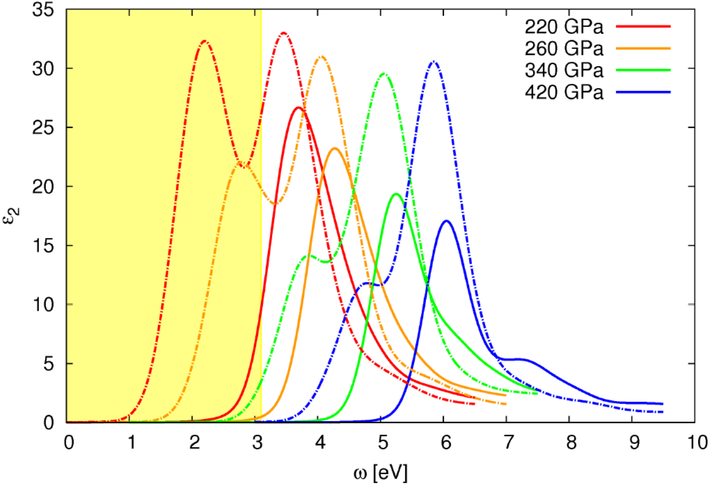

M.Gatti et al, Physical Review Letter **104**, 216404 (2010).

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Ab initio Spectroscopy Codes in the ETSF

- Abinit (DFT+GW `www.abinit.org`)
- DP (TDDFT in linear and non-linear response `www.dp-code.org`)
- Octopus (DFT and TDDFT in linear and non-linear response `www.tddft.org/programs/octopus`)
- EXC (BSE `www.bethe-salpeter.org`)
- Yambo (TDDFT and BSE `www.yambo-code.org`)