Optical properties from Elk code

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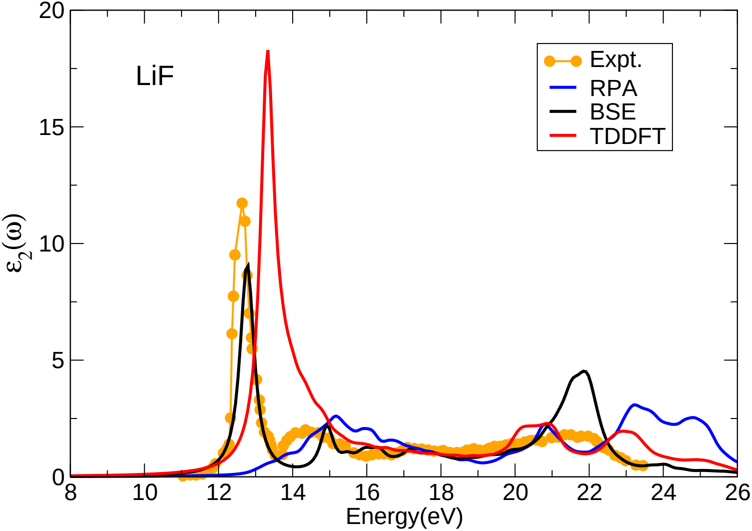
20 July 2011

Aim: Linear optical spectra of LiF



Linear optics: RPA

$$\varepsilon^{xy} = \sum_{vc\mathbf{k}} \frac{P^x_{vc\mathbf{k}} (P^y)^*_{vc\mathbf{k}}}{(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}} - \omega + i\eta)(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}})^2}$$

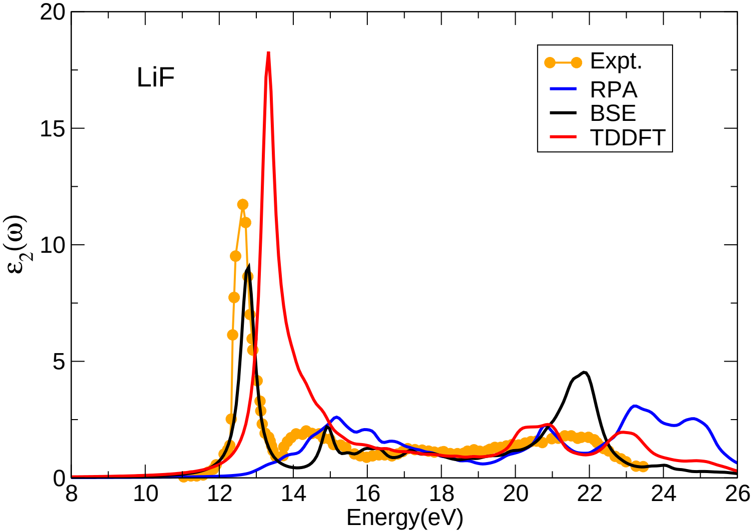
ϵ: ground state eigen values (task=0)
P^x: momentum matrix elements (task=120)
ε^{xy}: dielectric tensor with RPA (task=121)
Results in EPSILON-11.OUT

Important input parameters

$$\varepsilon^{xy} = \sum_{vc\mathbf{k}} \frac{P^x_{vc\mathbf{k}} (P^y)^*_{vc\mathbf{k}}}{(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}} - \omega + i\eta)(\epsilon_{v\mathbf{k}} - \epsilon_{c\mathbf{k}})^2}$$

number of **k**-points: ngridk
number of Kohn-Sham states v and c: nempty

Aim: BSE optical spectra of LiF



BSE

$$\varepsilon^{xy} = \sum_{\lambda} \left| \sum_{v c \mathbf{k}} A^{\lambda}_{v c \mathbf{k}} \frac{P^{x}_{v c \mathbf{k}} (P^{y})^{*}_{v c \mathbf{k}}}{\epsilon_{c\mathbf{k}} - \epsilon_{v\mathbf{k}}} \right|^{2} \left(\frac{1}{E^{\lambda} - \omega - i\eta} + \frac{1}{E^{\lambda} + \omega + i\eta} \right)$$

BSE matrix:

$$M_{vv'cc'\mathbf{k}\mathbf{k}'} = -\int d^3r d^3r' \phi_{v\mathbf{k}}(\mathbf{r}) \phi^{*}_{c\mathbf{k}}(\mathbf{r}') W(\mathbf{r},\mathbf{r}') \phi^{*}_{v'\mathbf{k}'}(\mathbf{r}) \phi_{c'\mathbf{k}'}(\mathbf{r}')$$

$$W(\mathbf{r},\mathbf{r}') = \frac{1}{\Omega} \sum_{\mathbf{G}\mathbf{G}'\mathbf{q}} e^{-i(\mathbf{G}+\mathbf{q}).\mathbf{r}} \frac{4\pi\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{|\mathbf{G}+\mathbf{q}||\mathbf{G}'+\mathbf{q}|} e^{i(\mathbf{G}'+\mathbf{q}).\mathbf{r}'}$$

ϵ: ground state eigen values (task=0)
P^{x}: momentum matrix elements (task=120)
$\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})$: inverse dielectric matrix (task=180)
E^{λ} and A^{λ}: BSE eigenvalues and eigenvectors (task=185)
Results in EPSILON-BSE-11.OUT

Important input parameters

$$W(\mathbf{r},\mathbf{r}') = \frac{1}{\Omega}\sum_{\mathbf{G}\mathbf{G}'\mathbf{q}} e^{-i(\mathbf{G}+\mathbf{q}).\mathbf{r}} \frac{4\pi\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{|\mathbf{G}+\mathbf{q}||\mathbf{G}'+\mathbf{q}|} e^{i(\mathbf{G}'+\mathbf{q}).\mathbf{r}'}$$

number of **G**-vectors: ngrpa
number of **q**-points=**k**-points: ngridk

$$M_{vv'cc'\mathbf{k}\mathbf{k}'} = -\int d^3r d^3r' \phi_{v\mathbf{k}}(\mathbf{r})\phi^*_{c\mathbf{k}}(\mathbf{r}')W(\mathbf{r},\mathbf{r}')\phi^*_{v'\mathbf{k}'}(\mathbf{r})\phi_{c'\mathbf{k}'}(\mathbf{r}')$$

number of valence states v: nvbse
number of conduction states c: ncbse

Important input parameters

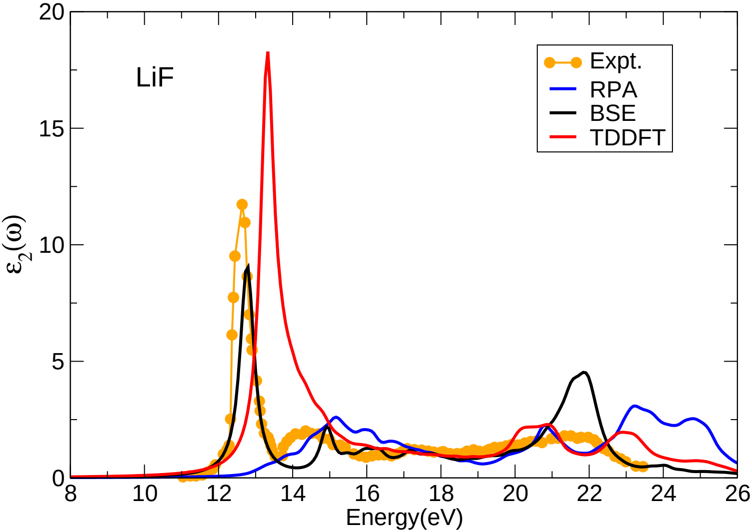
$$W(\mathbf{r},\mathbf{r}') = \frac{1}{\Omega}\sum_{\mathbf{G}\mathbf{G}'\mathbf{q}} e^{-i(\mathbf{G}+\mathbf{q}).\mathbf{r}} \frac{4\pi\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})}{|\mathbf{G}+\mathbf{q}||\mathbf{G}'+\mathbf{q}|} e^{i(\mathbf{G}'+\mathbf{q}).\mathbf{r}'}$$

number of **G**-vectors: ngrpa
number of **q**-points=**k**-points: ngridk

$$M_{vv'cc'\mathbf{k}\mathbf{k}'} = -\int d^3r d^3r' \phi_{v\mathbf{k}}(\mathbf{r})\phi^*_{c\mathbf{k}}(\mathbf{r}')W(\mathbf{r},\mathbf{r}')\phi^*_{v'\mathbf{k}'}(\mathbf{r})\phi_{c'\mathbf{k}'}(\mathbf{r}')$$

number of valence states v: nvbse
number of conduction states c: ncbse

Aim: TDDFT optical spectra of LiF



TDDFT

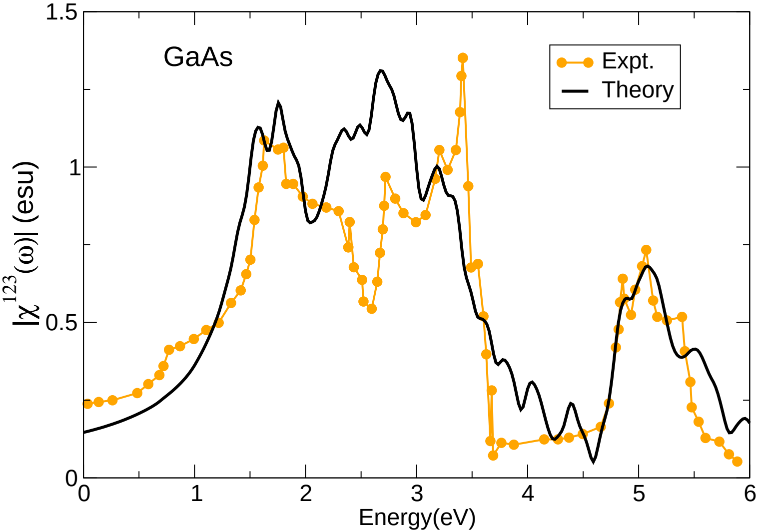
$$\varepsilon^{-1}(\mathbf{q},\omega) = 1 + v(\mathbf{q})\chi(\mathbf{q},\omega) = 1 + \frac{v(\mathbf{q})\chi_0(\mathbf{q},\omega)}{1 - \left[v(\mathbf{q}) + f_{\rm xc}(\mathbf{q},\omega)\right]\chi_0(\mathbf{q},\omega)},$$

where all quantities are matrices in the basis of reciprocal lattice vectors $\mathbf{G}$ for example in the optical limit $(\mathbf{q} \to 0)$ we want to plot

$$\varepsilon_{00}(\omega) = \left[\frac{1}{\varepsilon^{-1}_{\mathbf{G},\mathbf{G}'}(\mathbf{q} \to 0, \omega)}\right]_{\mathbf{G}=\mathbf{G}'=0}$$

$\chi_0 = 1 - v\varepsilon_0$: ground state eigen values (task=0)
P^x: momentum matrix elements (task=120)
$\varepsilon^{-1}_{\mathbf{G}\mathbf{G}'}(\mathbf{q})$: inverse dielectric matrix (task=188)
Results in EPSILON-TDDFT.OUT

Aim: SHG in GaAs



Second harmonic generation

$$\chi^{123}(\omega) = \sum_{nml\mathbf{k}} \frac{2P^1_{nm\mathbf{k}}P^2_{ml\mathbf{k}}P^3_{ln\mathbf{k}}}{(\epsilon_{ln\mathbf{k}} - \epsilon_{ml\mathbf{k}})(\epsilon_{mn\mathbf{k}} - 2\omega)} \cdots$$

$\epsilon_{nm} = \epsilon_n - \epsilon_m$: ground state Khon-Sham eigenvalues (task=0)
P^1_{nm}: momentum matrix elements (task=120)
χ: SHG susceptibility (task=123)
Results in CHI-123.OUT

Important parameter
number of **k**-points: ngridk
number of Kohn-Sham states n,m and l: nempty

Second harmonic generation

$$\chi^{123}(\omega) = \sum_{nml\mathbf{k}} \frac{2P^1_{nm\mathbf{k}}P^2_{ml\mathbf{k}}P^3_{ln\mathbf{k}}}{(\epsilon_{ln\mathbf{k}} - \epsilon_{ml\mathbf{k}})(\epsilon_{mn\mathbf{k}} - 2\omega)} \cdots$$

$\epsilon_{nm} = \epsilon_n - \epsilon_m$: ground state Khon-Sham eigenvalues (task=0)
P^1_{nm}: momentum matrix elements (task=120)
χ: SHG susceptibility (task=123)
Results in CHI-123.OUT

Important parameter
number of **k**-points: ngridk
number of Kohn-Sham states n,m and l: nempty