TDDFT: bootstrap approximation for the exchange-correlation kernel

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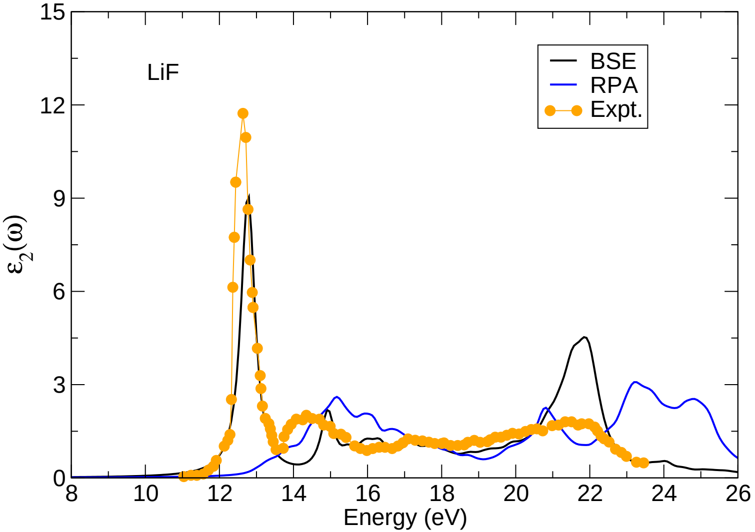
state of the art: GW+BSE



Bootstrap functional

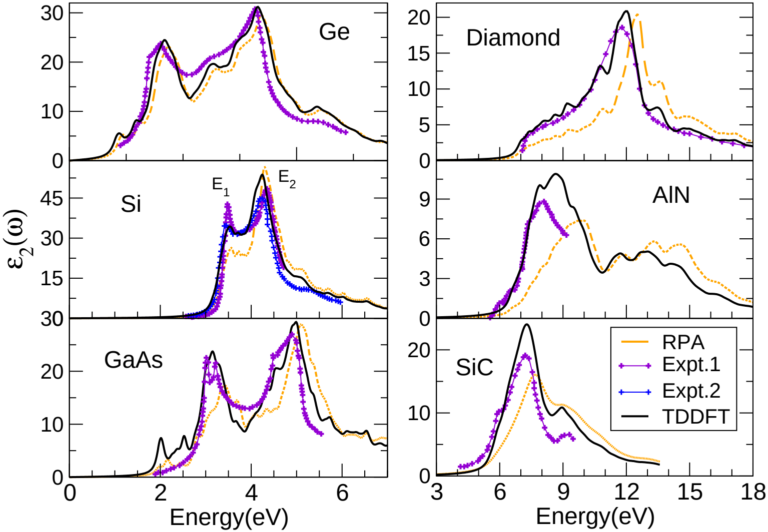
Dyson equation:

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

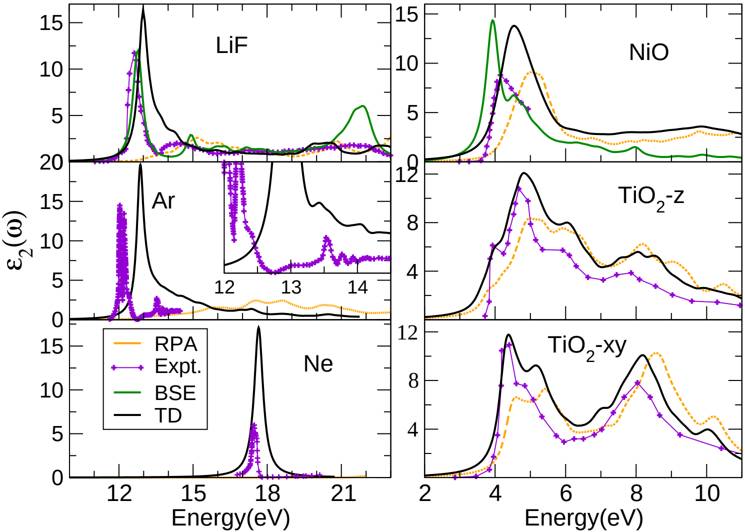
Bootstrap kernel

$$f_{\mathrm{xc}}^{\mathrm{BS}}(\mathbf{q},\omega) = -\frac{\varepsilon^{-1}(\mathbf{q},\omega=0)v(\mathbf{q})}{\varepsilon_0(\mathbf{q},\omega=0) - 1}$$

Small to medium bandgap material



Large bandgap insulators



Relation of Bootstrap to other functionals

Bootstrap kernel

$$f_{\mathrm{xc}}^{\mathrm{BS}}(\mathbf{q},\omega) = -\frac{\varepsilon^{-1}(\mathbf{q},\omega=0)v(\mathbf{q})}{\varepsilon_0(\mathbf{q},\omega=0)-1}$$

Two other functionals that work

1. LRC$=\frac{\alpha}{q^2}$

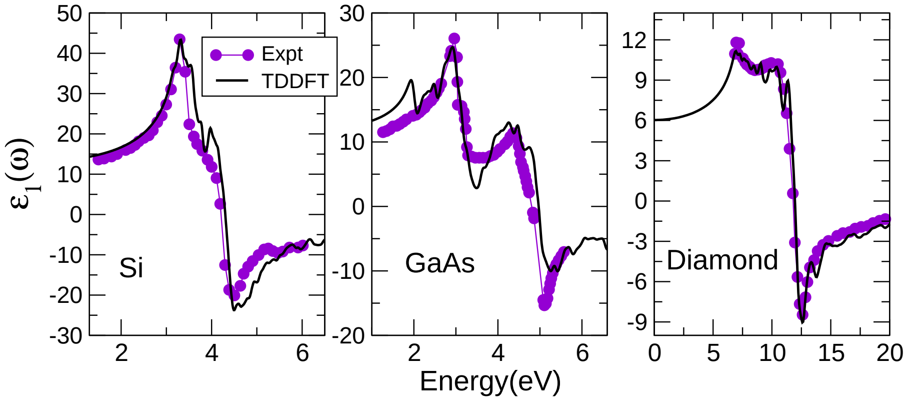
$$\left[-\frac{\varepsilon^{-1}(\mathbf{q},\omega=0)}{\varepsilon_0(\mathbf{q},\omega=0)-1}\right]v(\mathbf{q}) = \left[-\frac{\varepsilon^{-1}(\mathbf{q},\omega=0)}{\varepsilon_0(\mathbf{q},\omega=0)-1}\right]\frac{4\pi}{q^2}$$

2. BSE derived NQ kernel

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

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

Real part of the dielectric function



Importance of bootstrap procedure