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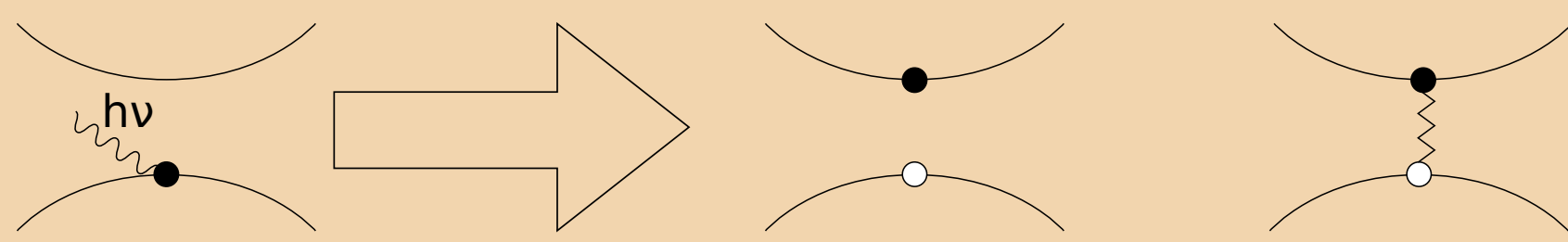
# Ab initio study of Silver chloride: Modelization of the dielectric function

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## Bethe-Salpeter equation



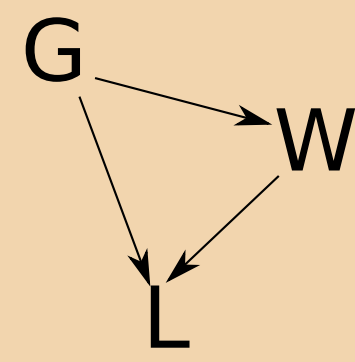
Optical calculation needs to take into account the screened electron hole to be correct. The usual way to do this is to use the Bethe Salpeter equation (BSE).

$$L = L_0 + L_0 K L$$

But

-Complex equation: two particles ! Long computation → Haydock algorithm

-Need to compute the screening W ! Even longer... → Can we try to model it ? Yes !  $W = \epsilon^{-1} v$



$$\epsilon = 1 + \frac{1}{\frac{1}{\epsilon_{\infty} - 1} + \alpha \left( \frac{q}{q_{TF}} \right)^2 + \frac{q^4}{4m\omega_p^2}}$$

$\omega_p = \sqrt{4\pi\rho}$  is the plasma frequency of the system,  $q_{TF} = 2 \left( \frac{3\rho}{\pi} \right)^{1/6}$  is the Thomas Fermi wave-vector.  $\alpha = 1.563$  is a fixed parameter, it is set by a best fit on different materials.  $\rho$  is the average density of the material.

$\epsilon_{\infty}$  is the dielectric constant of the material → It has to be computed.

With this model we only have one value to compute !

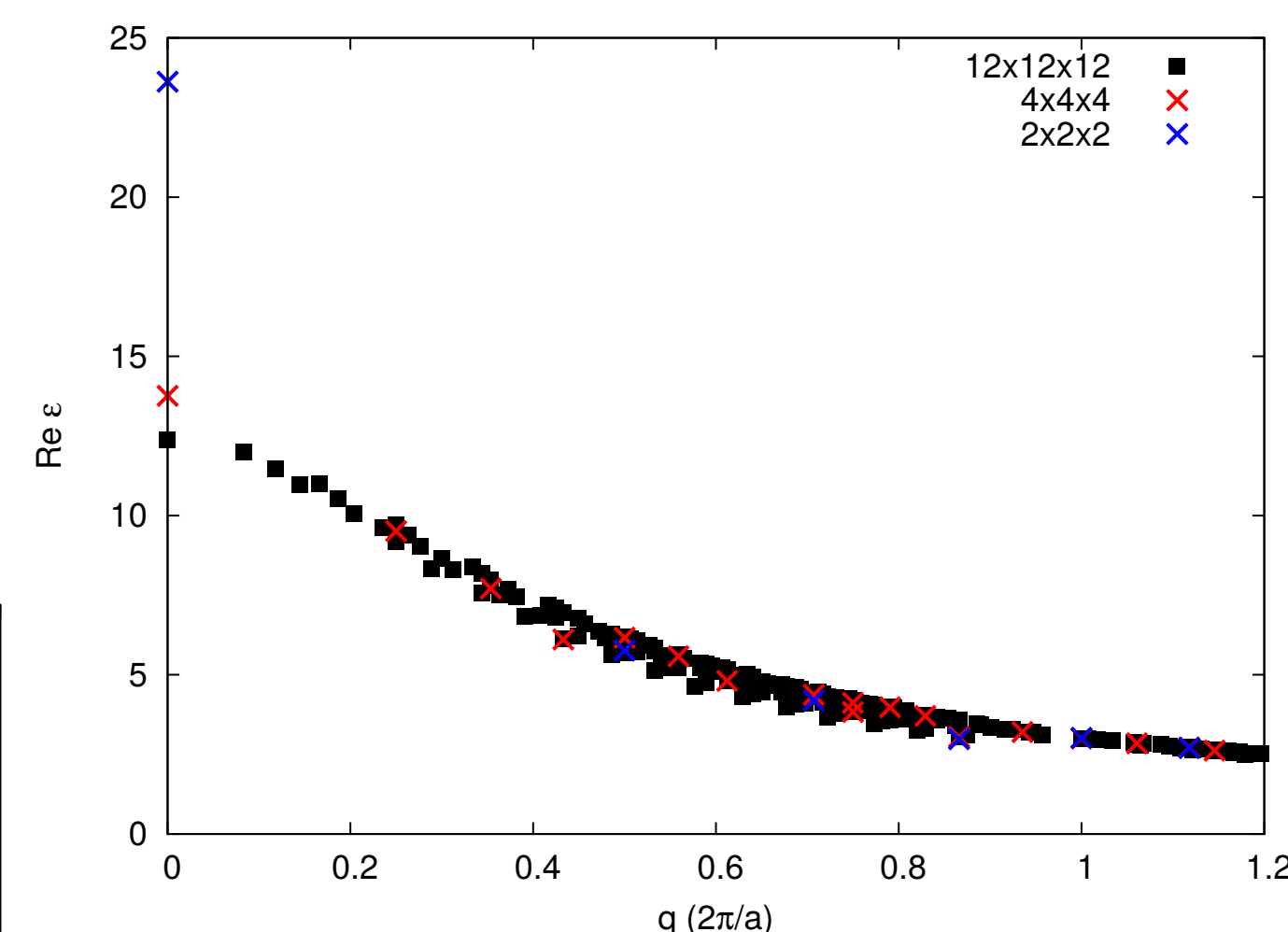
Is this model helpful ? How does the screening behave with convergence of parameters ?

Cappellini, G.; Del Sole, R.; Reining, L. & Bechstedt, F. Phys. Rev. B, 1993

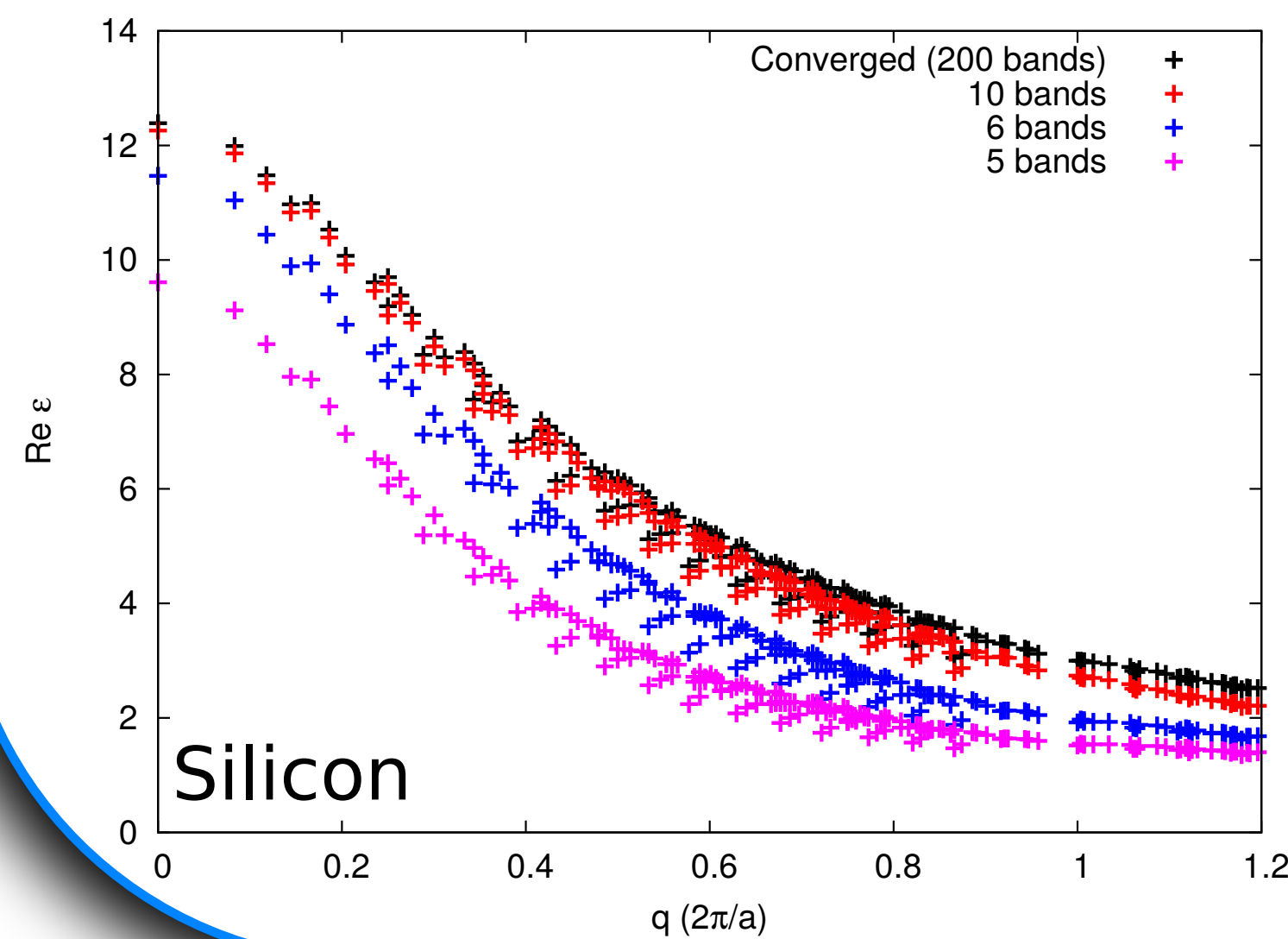
## Convergence with the size of the grid and the numbers of bands

The effect of different parameters on the screening has been studied.

First, different grids of k points have been tested. We see that the screening is well converged for large q but is not converged for vanishing q. Then it will require more effort to compute the dielectric constant.



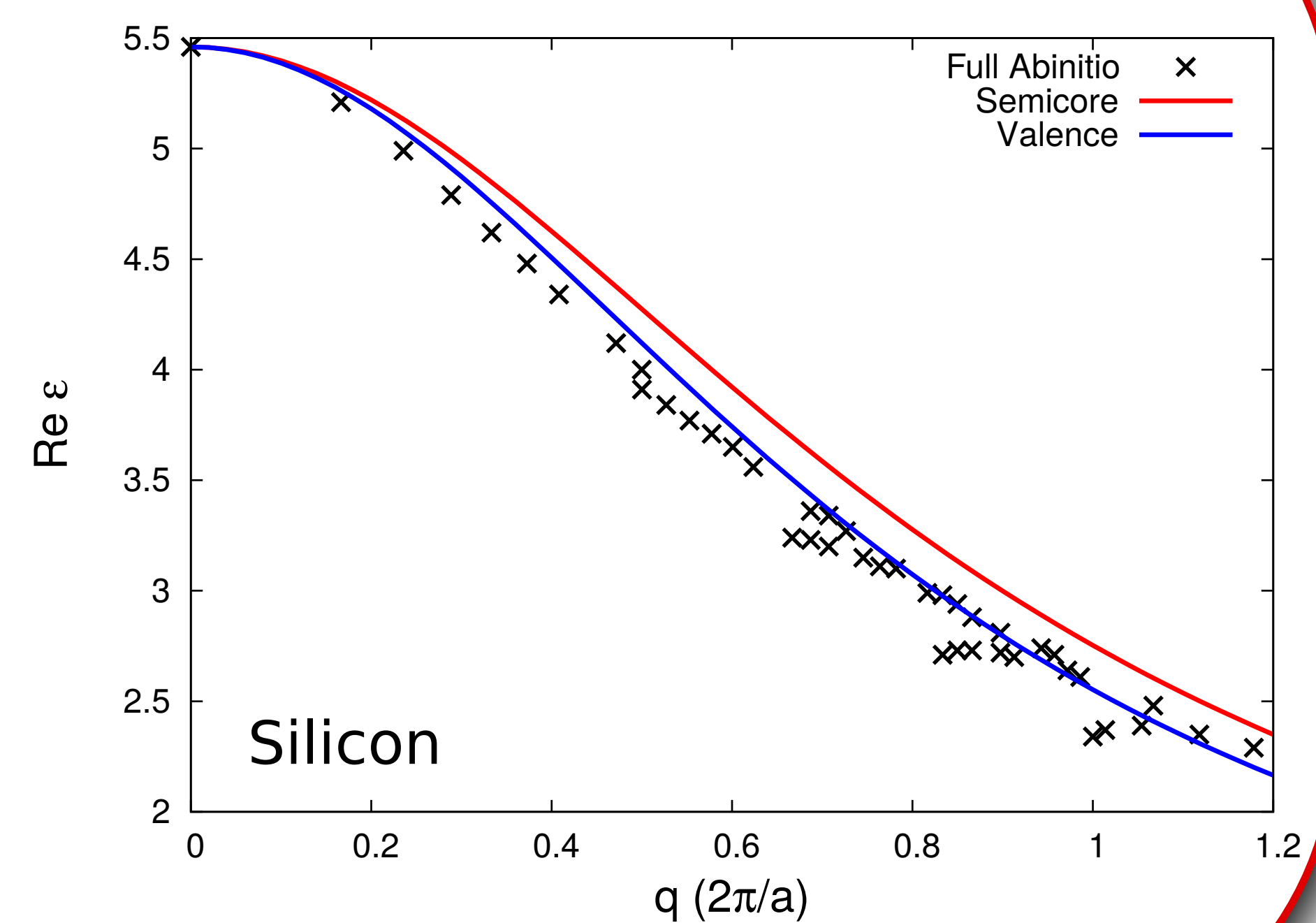
Second, screening with a different number of bands has been computed. In this case no q point converges faster than the others. So this parameter will have to be correctly converged in any case.



## Density ?

The model includes the average density of the material. But which density ? For a material like silver chloride with semicore states, which states shall be included ?

Comparing models using both densities, we see that using only the valence state is a more accurate choice.



## Using another q

According to previous points, the dielectric function at q=0 is a more difficult point to compute than dielectric function at other momentum.

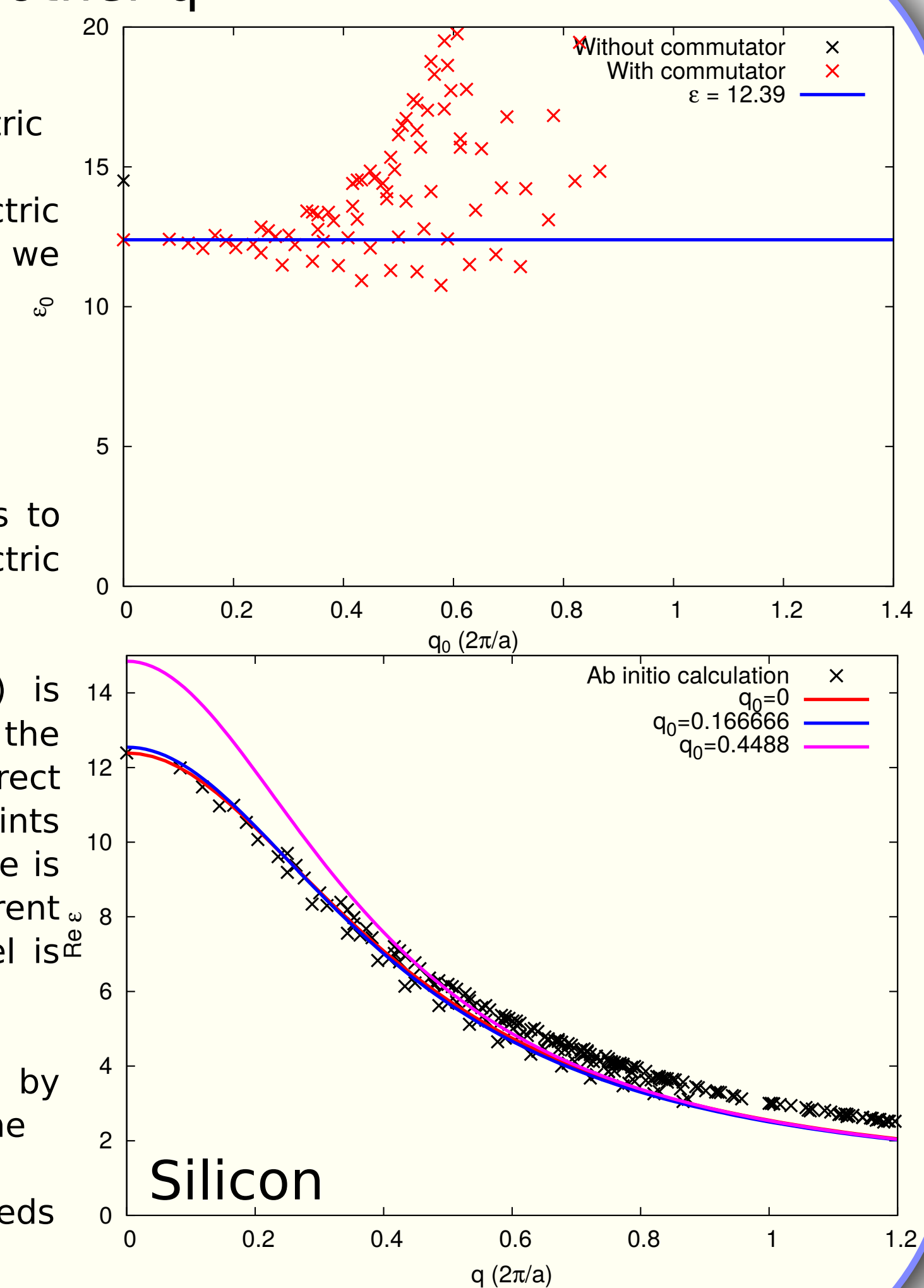
One can wonder if it can use another value of the dielectric function to define the model. This is indeed possible, if we rewrite the equation for the model:

$$\epsilon(q) = 1 + \frac{1}{\frac{1}{\epsilon(q_0) - 1} + \alpha \left( \frac{q^2 - q_0^2}{q_{TF}^2} \right) + \frac{q^4 - q_0^4}{4\omega_p^2}}$$

Where  $\epsilon(q_0)$  is the dielectric function at  $q_0$ . This allows to only compute  $\epsilon(q_0)$  instead of  $\epsilon(q \rightarrow 0)$  and get the dielectric function at all q.

To check if this can be used, the value of  $\epsilon(q > 0)$  is computed for each choice of  $q_0$ . The result is plotted on the top figure. We see that obviously  $q_0 \rightarrow 0$  give the correct result and that, small  $q_0$  gives correct result while the points rapidly diverge to incorrect values. On the bottom figure is plotted the model dielectric function generated by different  $q_0$  points. We see that for small value of  $q_0$  the model is indeed correct, but become bad for large values of  $q_0$ .

→ Using another q point to define the model is favored by computational time consideration (commutator, size of the grid) but is limited by the model itself as it increases the error made by the approximation (anisotropy,...) and needs a small value of transferred momentum to be correct.

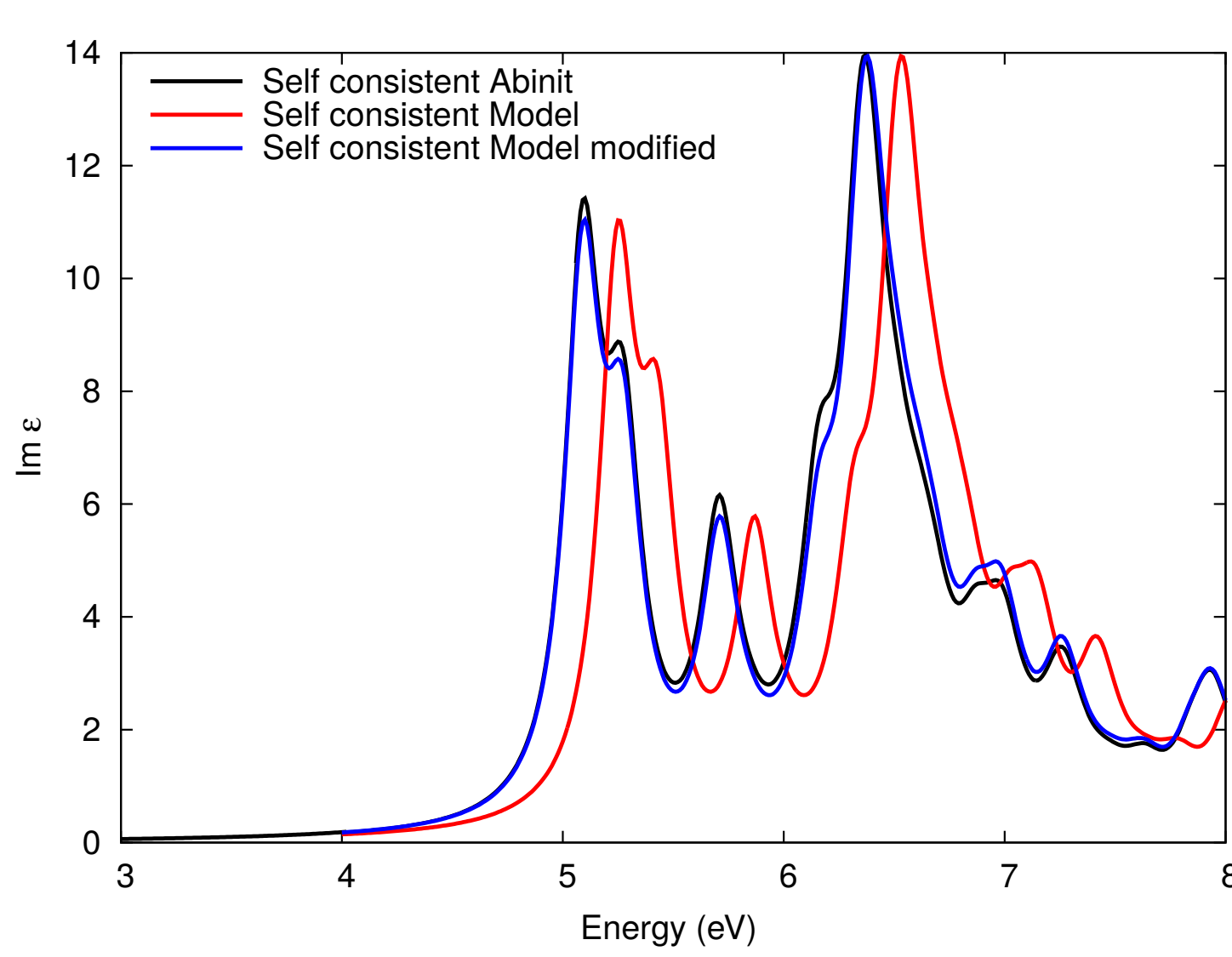
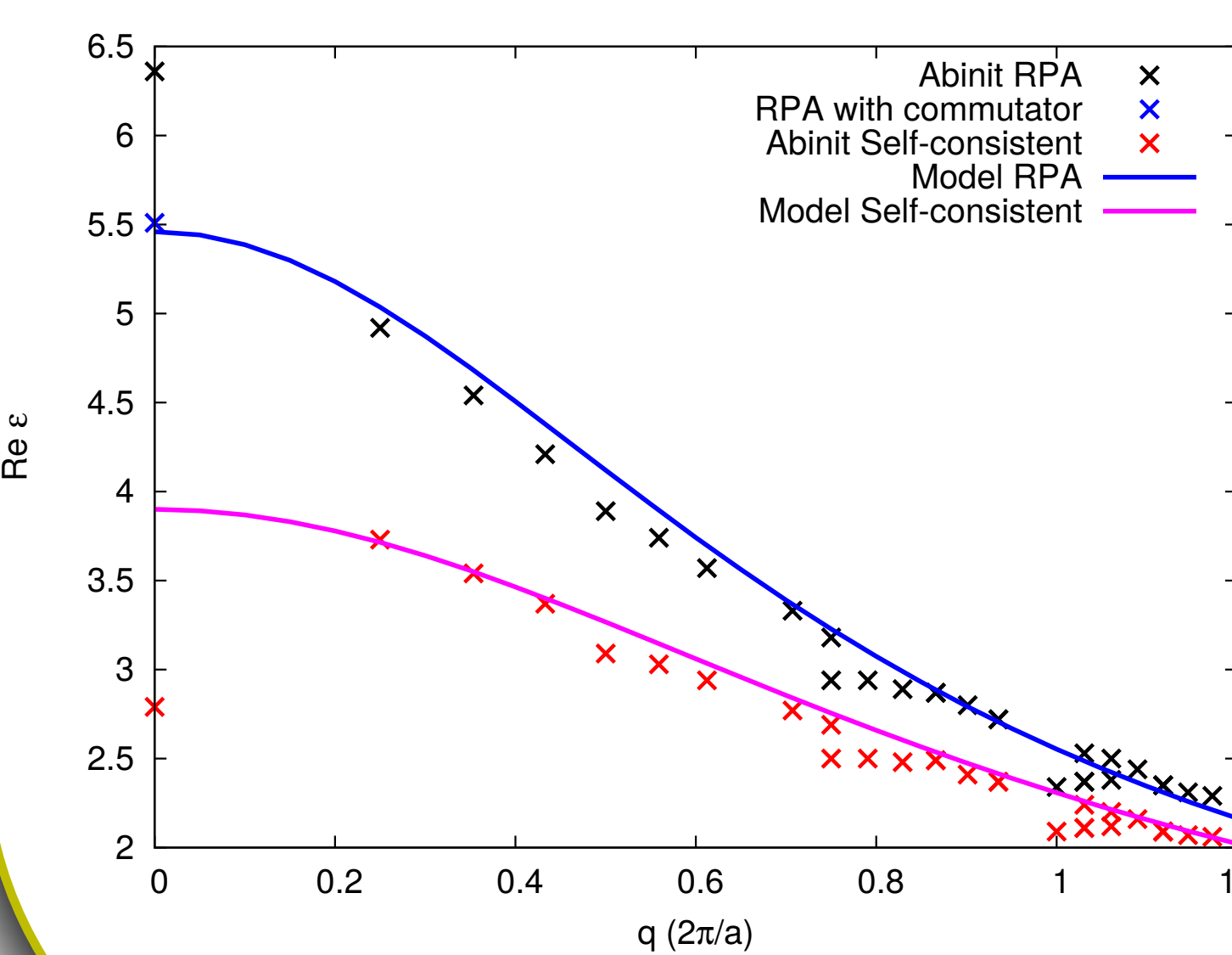
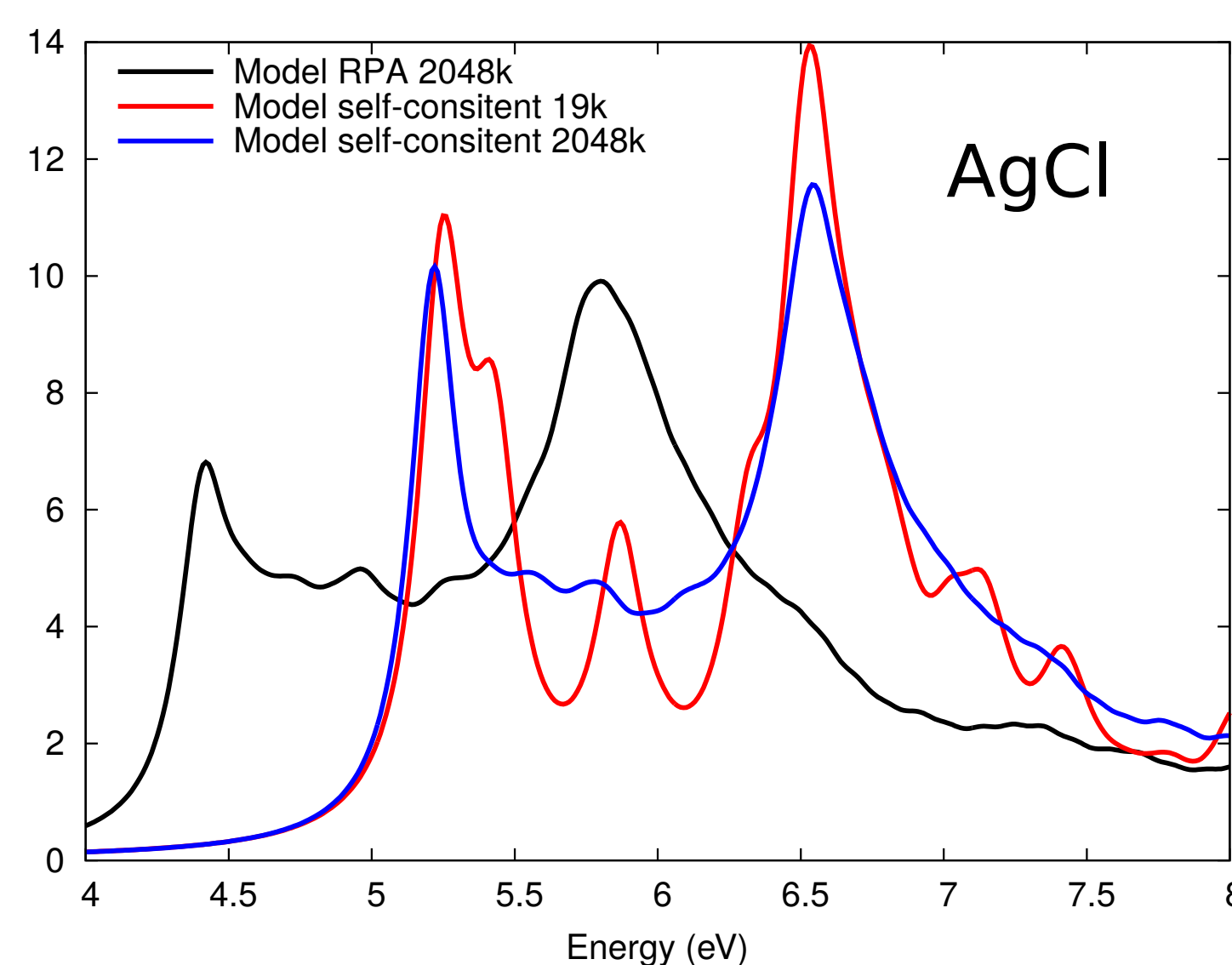


## Applying the model

With this model we can now make a faster calculation or even calculation that was not achievable.

Here the model has been used to extrapolate the screening for different grids. This avoids the calculation of a screening for every grid whereas the screening is already converged. This is applied to converge BSE calculation on top of a G0W0.

We can also use the model to correct the error on some particular q. For example in a self consistent GW calculation with an incorrect dielectric constant (red points below) we can estimate the dielectric constant and get a "corrected" model. This in turn allows calculation on finer grid. Something that would not have been possible for a self consistent calculation without model.



## Conclusion

We have studied here a model for the dielectric function and applied it to the computation of BSE on top of a self consistent GW calculation.

The model only needs one value of the dielectric function but one should be careful with the computation of this value as it will affect the whole model dielectric function. We have seen on this poster the example of the commutator and the input density.

Using another value of the dielectric function as input for the model is possible but this value has to be computed for a small  $q_0$ , meaning a fine grid to compute it, removing value as time saving technique.

Finally, the model brings several advantages:

- Only one value of the dielectric function needs to be calculated, instead of a calculation on a whole grid to get the result for a given grid. It could be at vanishing momentum or at close to zero momentum.

- The screening can be calculated for any momentum and thus for any grid, even for random grid.
- Starting with a calculated screening on a small grid, the model can extend it to larger grid, even if the dielectric constant of the smaller grid is not correct.