Linear response of the bulk gold

kick field: $A_{ext} = A_0\,\theta(t), \quad E_{ext} = E_0\,\delta(t)$

Dielectric function: $\varepsilon = \frac{D(\omega)}{E(\omega)} = \frac{E_{ext}(\omega)}{E_{tot}(\omega)} = \frac{E_{ext}(\omega)}{E_{ext}(\omega)+E_{ind}(\omega)}$

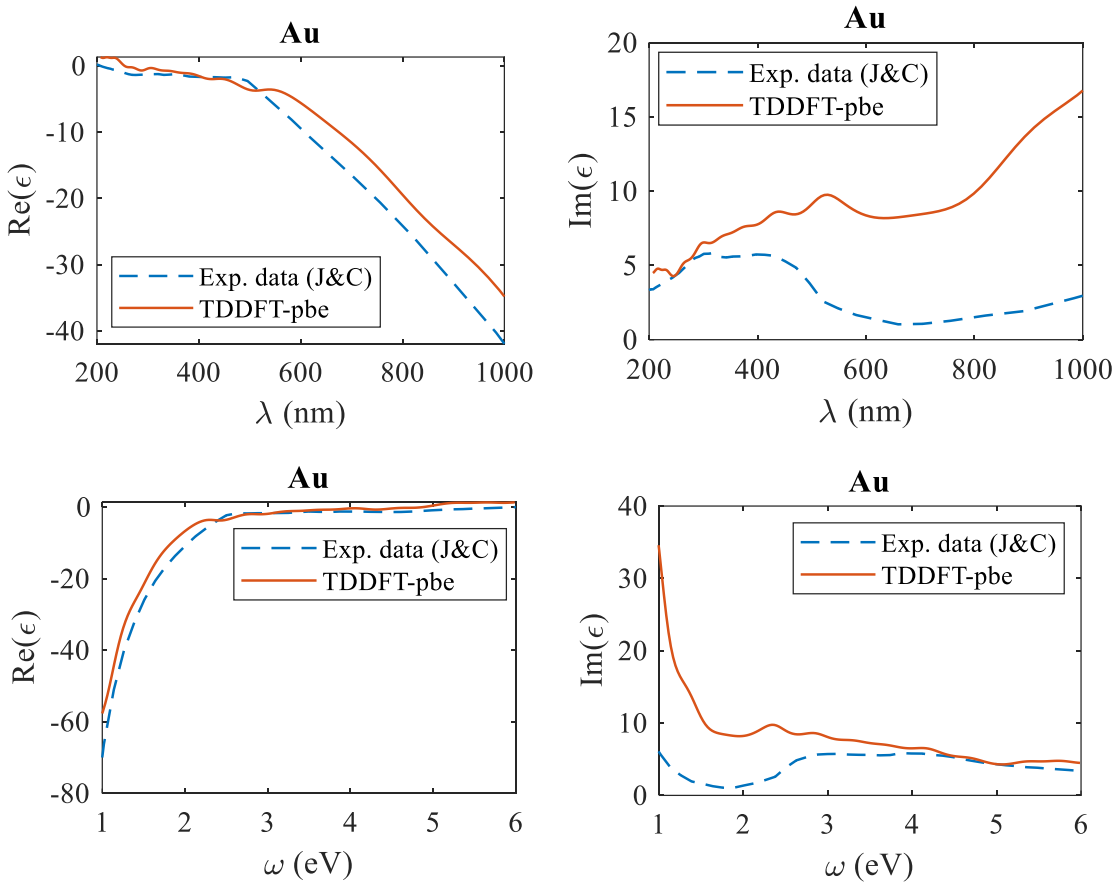
Calculation detail: Pseudopotential and XC: PBE k-points=20×20×20

Smearing function: Fermi-Dirac (0.1 eV) Grid spasing: 0.4 a.u.

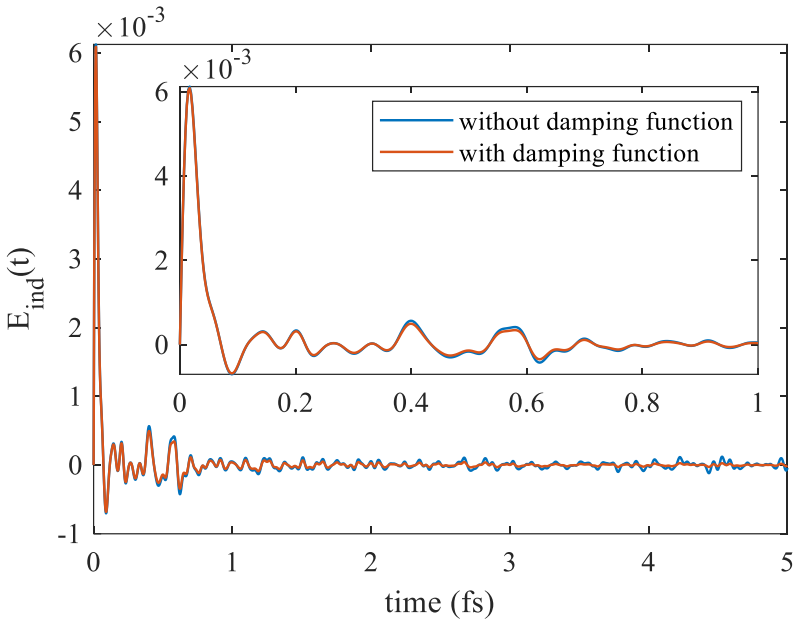
Propagation time: 413 a.u.=10 fs time-step: 0.1 a.u.

Results

Dielectric function (ε)



Induced electric field (E_{ind}) of the bulk gold



Band structure of the bulk gold