**Far-field Properties**[1,2]. Extinction spectra are calculated by integrating the time-averaged extinction Poynting vectors $\boldsymbol{S_{ext}}$ (i.e. electromagnetic power flow) over an auxiliary surface enclosing the Au NP dimer or the isoalted NP:

$$\boldsymbol{S}_{ext} = \frac{1}{2}\mathrm{Re}\{\boldsymbol{E}_{inc} \times \boldsymbol{H}_{sca}{}^{*} + \boldsymbol{E}_{sca} \times \boldsymbol{H}_{inc}{}^{*}\} \quad (1)$$

$$C_{ext} = \frac{-\iint \boldsymbol{S}_{ext} d\mathrm{A}}{|\mathbf{W}_{inc}|} \quad (2)$$

where $\boldsymbol{E}_{\mathrm{inc}}$, $\boldsymbol{E}_{\mathrm{sca}}$, $\boldsymbol{H}_{\mathrm{inc}}$ and $\boldsymbol{H}_{\mathrm{sca}}$ are the incident and scattered electric and magnetic field respectively, $\boldsymbol{C}_{ext}$ is the extinction cross section, $|\mathbf{W}_{inc}| = {}^{1}/_{2}\, c\varepsilon_0 \mathrm{E}_0{}^{2}$ is the power flow per unit area of the incident plane wave, $E_0$ (set at 1 V/m here) is the modulus of $\boldsymbol{E}_{\mathrm{inc}}$, $c$ is the velocity of light and $\varepsilon_0$ is the permittivity of vacuum.