Electronic Supplementary Information (ESI) for

Small Morphology Variations Effects on Plasmonic Nanoparticle Dimer Hotspots

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Far-field extinction spectra

The calculated far-field extinction spectra of the bridged, creviced, faceted and roughened dimers are plotted in Fig. S1-S4. They are calculated by integrating the time-averaged extinction Poynting vectors $\boldsymbol{S}_{\text{ext}}$ (i.e. electromagnetic power flow) over an auxiliary surface A enclosing the dimer, respectively:[1]

$$S_{ext} = \frac{1}{2} Re\left\{E_{inc} \times {H_{sca}}^{*} + E_{sca} \times {H_{inc}}^{*}\right\} \quad \text{(S1)}$$

$$C_{ext} = \frac{-\iint S_{ext} dA}{|W_{inc}|} \quad \text{(S2)}$$

where $\boldsymbol{E}_{inc}$, $\boldsymbol{E}_{sca}$, $\boldsymbol{H}_{inc}$ and $\boldsymbol{H}_{sca}$ are the incident and scattered electric and magnetic field respectively. C_{ext} is the extinction cross section, $|W_{inc}| = {}^{1}/_{2} c\varepsilon_0 {E_0}^2$ is the power flow per unit area of the incident plane wave, E_0 (set at 1 V/m here) is the modulus of $\boldsymbol{E}_{inc}$, c is the velocity of light and ε_0 is the permittivity of vacuum.

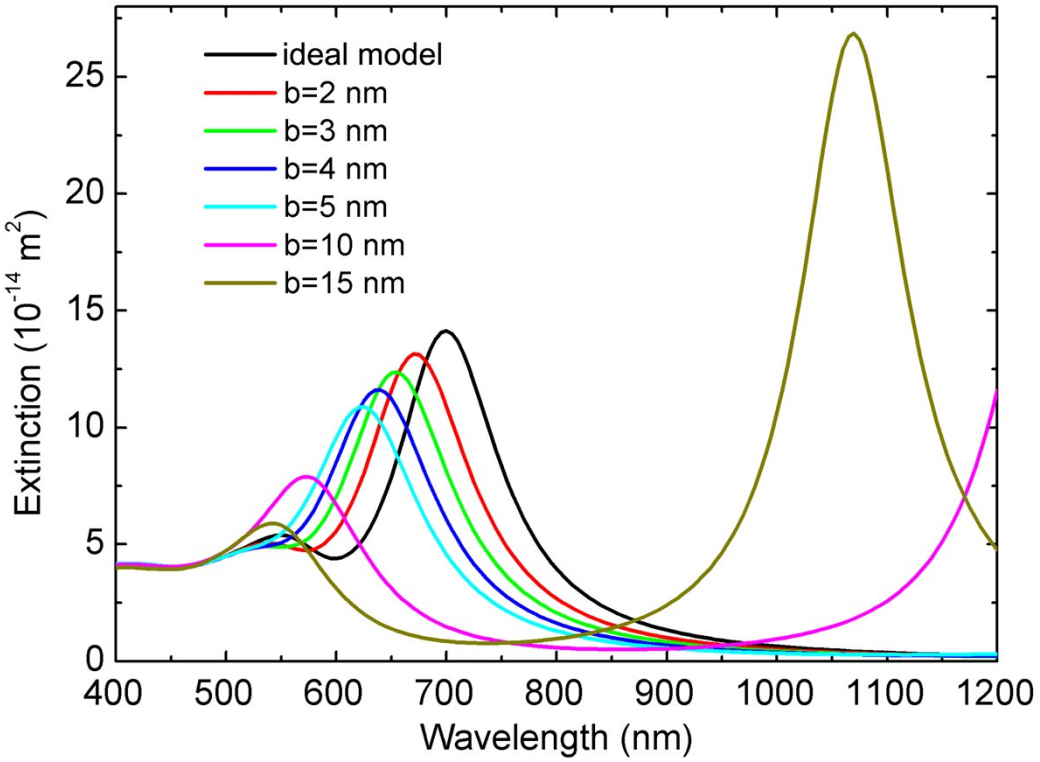

Figure S1. FEM calculated far-field extinction spectra for the bridge dimers as *b* is increased from 2 to 15nm, corresponding to Fig. 1.

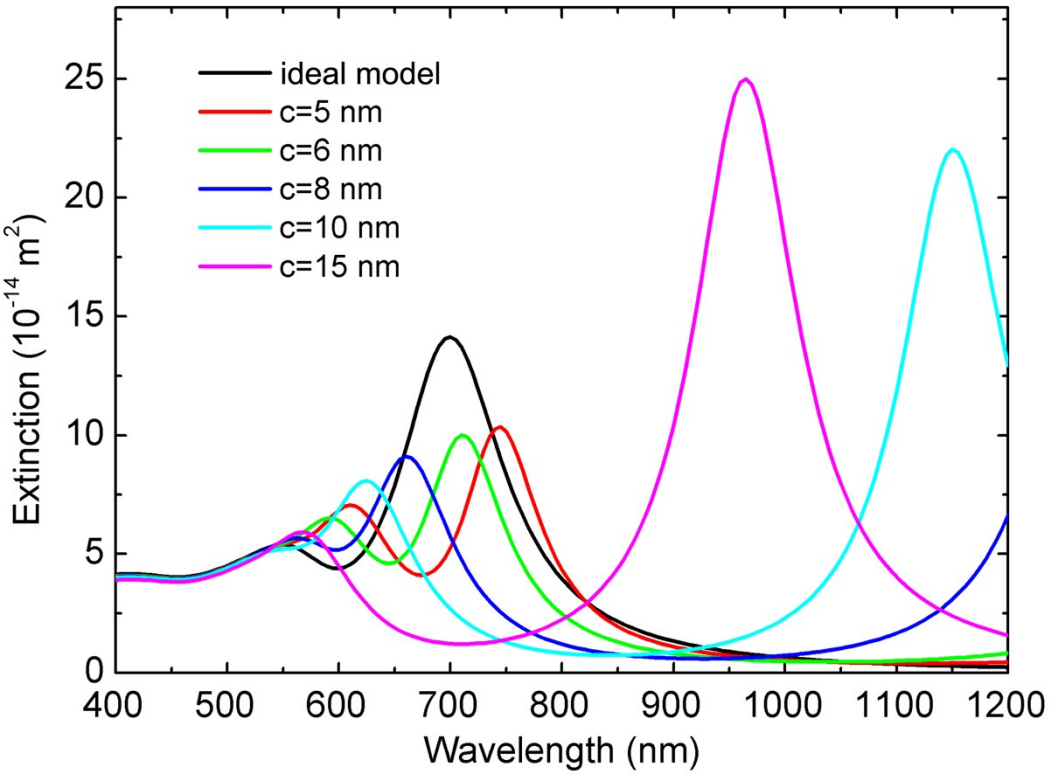

Figure S2. FEM calculated far-field extinction spectra for the creviced dimers as *c* is increased from 5 to 15nm, corresponding to Fig. 3.

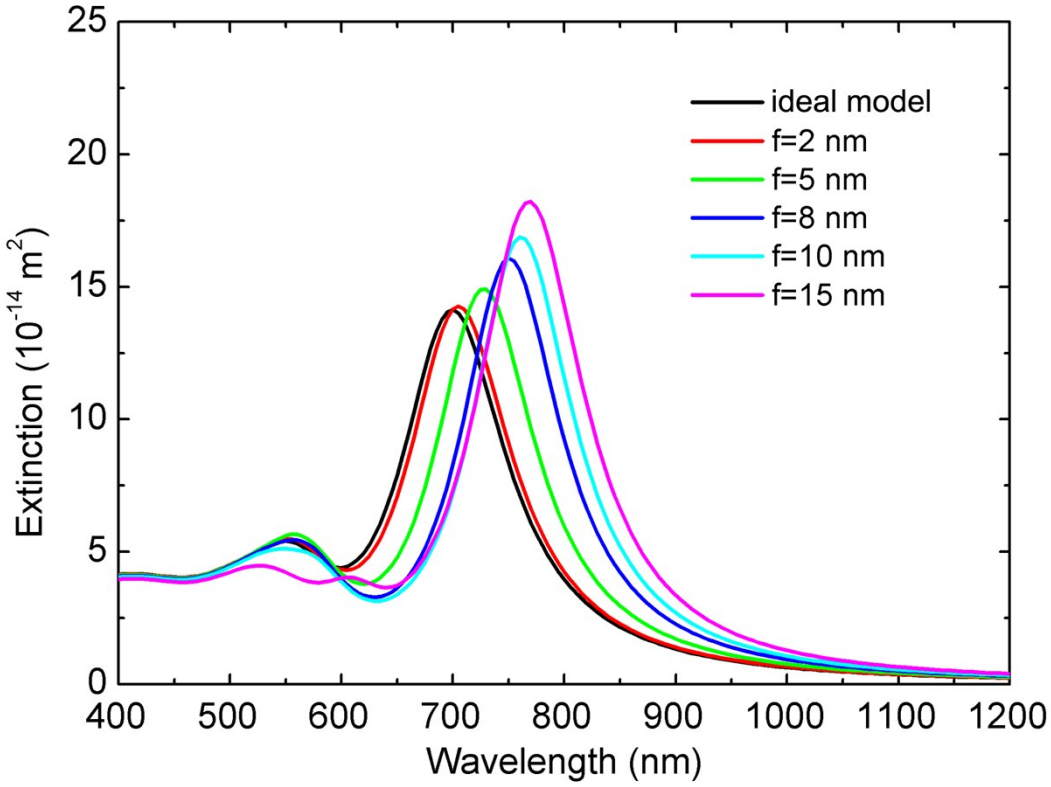

Figure S3. FEM calculated far-field extinction spectra for the faceted dimers as *f* is increased from 2 to 15nm, corresponding to Fig. 5.

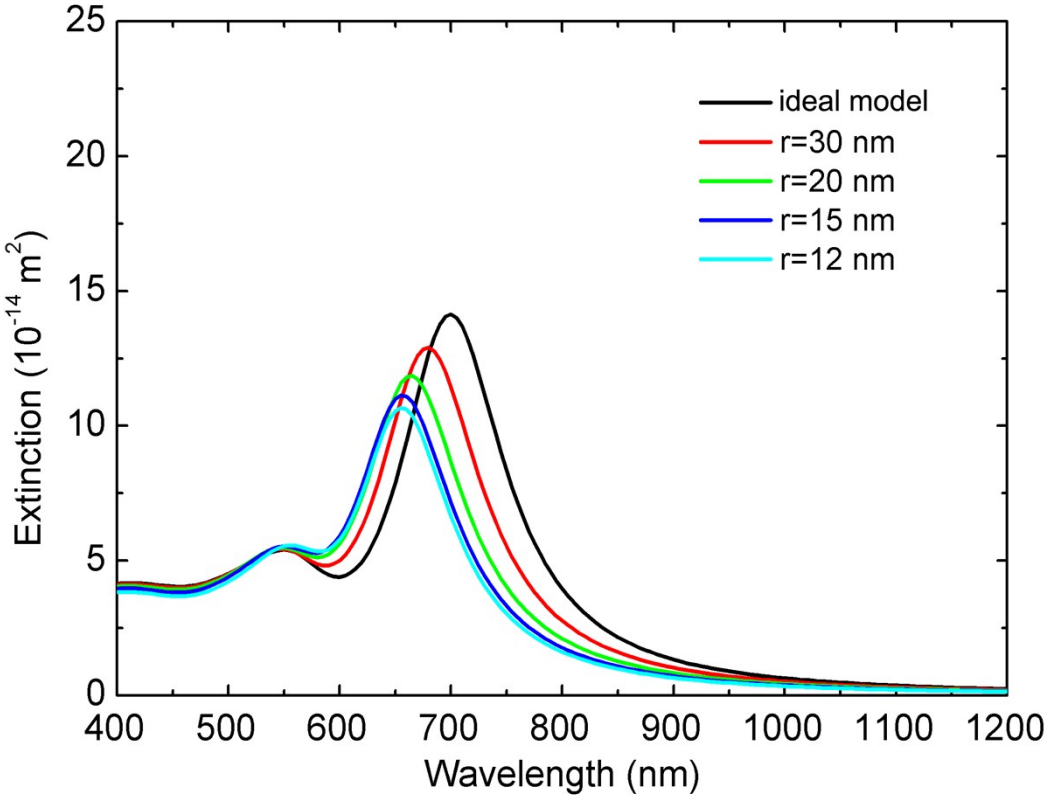

Figure S4. FEM calculated far-field extinction spectra for the roughened dimers as *r* is decreased from 30 to 12 nm, corresponding to Fig. 7.

Reference

1 V. Giannini, A. I. Fernandez-Dominguez, S. C. Heck and S. A. Maier, *Chem. Rev.*, 2011, **111**, 3888-3912.