## Variations of Plasmon Coupling between Two Identical Au Nanospheres with Their Separation and Sizes Studied within a Hibridization Scheme

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### Introduction

The plasmon coupling effect is studied using a simple scheme adapted from the quantum orbital hybridization model.



**Figure 1.** (a) Scheme of two identical metal nanospheres where *x* and *r* are separation and radius of spheres. (b) Plasmon hybridization model of (a)

#### **Basic Formulation**

Mimicking quantum mechanics formulation of linear combination of the two plasmon modes.

$$E_{\pm} = \frac{\alpha \pm \beta(x, r)}{1 \pm S(x, r)}$$

where

- α = LSPR energy of each uncoupled plasmon,
- $\succ \beta$  = the coupling parameter,
- $\succ$  S = the orbital overlap = 0

#### Results

The best fit with the set of coefficients (αi, bi, ci) given in Table 1 is obtained by the following expression

$$E_{-}^{i}(x) = \alpha_{i} \frac{b_{i}}{x^{2}} e^{\frac{c_{i}}{x}}$$

**Table 1.** Coefficients of bonding energyscheme for various radii

i	$r_i$ (nm)	α <sub>i</sub>	b <sub>i</sub>	C <sub>i</sub>
1	12	2.308	51.92	-11.97
2	16	2.296	150	2.05
3	20	2.281	329.6	15.66



**Figure 2.** Variation of bonding energy for increasing center-to-center separation for various radii of the Au nanospheres.

#### Conclusion

Hybridization scheme developed in this study shows that the interparticle coupling depends on the separation and the size of particles.

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