Supplementary information for

Plasmon Resonance Analysis with Configuration Interaction

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Case 2a: Vary α_1 only

We consider the case where only a single value of α is different from the others. We consider all values of β to be the same. The resulting matrix is:

$$\begin{bmatrix} \alpha_1 & \beta & \beta \\ \beta & \alpha & \beta \\ \beta & \beta & \alpha \end{bmatrix} \quad (1)$$

where $\alpha_1=\alpha+\varepsilon$. ε can be a positive or negative number. The eigenvalues for such a system are:

$E_1 = \alpha - \beta$, $E_2 = \alpha + \frac{1}{2}(\varepsilon + \beta) - \frac{1}{2}\sqrt{9\beta^2 - 2\beta\varepsilon + \varepsilon^2}$ and

$E_3 = \alpha + \frac{1}{2}(\varepsilon + \beta) + \frac{1}{2}\sqrt{9\beta^2 - 2\beta\varepsilon + \varepsilon^2}$.[55] We see that E_1 does not depend on ε and its value therefore remains constant. On the other hand, E_2 and E_3 both depend on ε.

We now analyze the peak oscillator strengths by considering numerical values for ε of ±0.05, ±0.25, ±0.5, ±1.0, ±1.5, ±2.0 and ±2.5 eV. This corresponds to changes in α_1 by ±1, ±5, ±10, ±20, ±30, ±40 and ±50% of the value used in case 1 (5 eV). All other matrix elements remain the same as in case 1 (β=0.5 eV and $\alpha_2= \alpha_3$= 5 eV). The resulting matrix is:

$$\begin{bmatrix} \alpha_1 & 0.5 & 0.5 \\ 0.5 & 5 & 0.5 \\ 0.5 & 0.5 & 5 \end{bmatrix} \quad (2)$$

where α_1= 2.5, 3.0, 3.5, 4.0, 4.5, 4.75, 4.95, 5.05, 5.25, 5.5, 6.0, 6.5, 7.0 and 7.5 eV. The peak energies E_i (i=1, 2, 3) and oscillator strengths S_i (i=1, 2, 3) are shown in Figure S1A and S1B respectively.

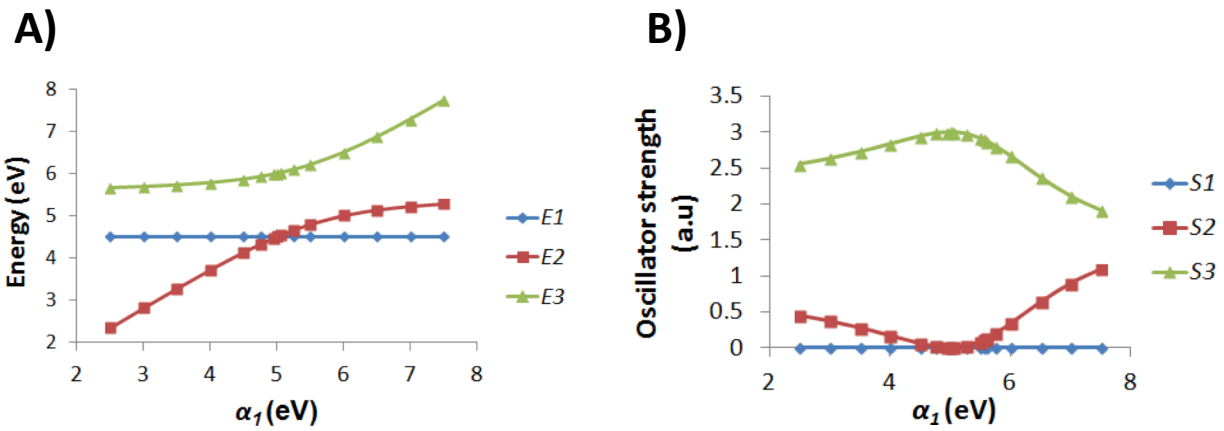

Figure S1. A) Peak energies and B) oscillator strengths for different values of α_1 (case 2a).

The computed values of the energy and oscillator strength are reported in Table S1. Just as in the ideal case, the high-energy excited state E_3 with high oscillator strength corresponds to the plasmon. We can see that the degeneracy between E_1 and E_2 is lifted when α_1 shifts away from the 5 eV value of case 1. This can be explained by the ε-dependence of E_2. For ε=0, E_2=E_1= 4.5 eV, which corresponds to the ideal case. E_1 remains at 4.5 eV (α-β) and does not depend on ε, as derived analytically, and its oscillator strength remains 0. We note that E_1 is larger than E_2 when α_1< 5eV and smaller than E_2 when α_1> 5eV. This is because these excited states are labeled to correspond to the analytical results and not by increasing energies. E_2 quickly rises when α_1 increases from 2.5 to 5.5 eV and then slowly stabilizes for higher values of α_1. On the other hand, E_3 slowly increases when α_1 shifts from 2.5 to 5.5 eV and quickly rises when α_1 is larger than 5.5 eV. The second and third eigenvalue expressions can be divided into two ε-dependent terms. The first term is $T_1 = \alpha + \frac{1}{2}(\varepsilon + \beta)$, which increases linearly with ε. This term is the same for both E_2 and E_3. The second term is $T_2 = \pm\frac{1}{2}\sqrt{9\beta^2 - 2\beta\varepsilon + \varepsilon^2}$. The plus sign is for E_3 and the negative sign is for E_2. The expression under the square root is quadratic. We note that the value

$\sqrt{9\beta^2 - 2\beta\varepsilon + \varepsilon^2}$ is always positive regardless of the value of ε since β is real. For the eigenvalue E_2, T_2 increases with increasing ε until it reaches its maximum value $\varepsilon = \beta = 0.5$. For $\varepsilon > \beta$, T_2 decreases. As a result, E_2 is expected to become larger until ε reaches the value of β. Due to the opposite sign of T_2, the opposite behavior is expected for E_3. E_3 therefore becomes larger with increasing ε when $\varepsilon > \beta$.

The values of T_1 and T_2 for the E_2 and E_3 peaks for the CI matrix given by eq. 2 are given in Tables S2 and S3. When α_1 increases from 2.5 to 5.5 eV, both T_1 and T_2 become larger and therefore E_2 does as well. When α_1 becomes larger than 5.5 eV ($\varepsilon > \beta$), T_2 starts to decrease and E_2 starts to stabilize. The peak at E_3 (the plasmon peak) shows the opposite behavior: its energy slowly increases when α_1 shifts from 2.5 to 5.5 eV ($\varepsilon < \beta$) and quickly rises when α_1 becomes larger than 5.5 eV, as explained by the opposite sign of T_2 in the analytical expression.

Table S1. Energies and oscillator strengths for varying values of α_1 (case 2a). Case 1 is shown in bold.

$\Delta\alpha_1$ (%)	α_1 (eV)	E_1 (eV)	S_1 (a.u.)	E_2 (eV)	S_2 (a.u.)	E_3 (eV)	S_3 (a.u.)
-50	2.5	4.5	0	2.3417	0.4448	5.6583	2.5552
-40	3.0	4.5	0	2.8139	0.3684	5.6861	2.6315
-30	3.5	4.5	0	3.2753	0.2752	5.7247	2.7248
-20	4.0	4.5	0	3.7192	0.1661	5.7808	2.8338
-10	4.5	4.5	0	4.134	0.0566	5.866	2.9433
-5	4.75	4.5	0	4.3246	0.0164	5.9254	2.9836
-1	4.95	4.5	0	4.4663	0.0007	5.9837	2.9991
0	**5.0**	**4.5**	**0**	**4.5**	**0.0000**	**6**	**3.0000**
1	5.05	4.5	0	4.533	0.0008	6.017	2.9991
5	5.25	4.5	0	4.6569	0.0203	6.0931	2.9798
10	5.5	4.5	0	4.7929	0.0858	6.2071	2.9142
20	6.0	4.5	0	5	0.1044	6.5	2.8958
30	6.5	4.5	0	5.134	0.1245	6.866	2.8751
40	7.0	4.5	0	5.2192	0.1945	7.2808	2.8056
50	7.5	4.5	0	5.2753	0.3334	7.7247	2.6664

Table S2. Values of T_1 and T_2 for the state with energy E_2 (case 2a).

α_1 (eV)	ε (eV)	E_2 (eV)	T_1 (eV)	T_2 (eV)
2.5	-2.5	2.3417	4.0000	-1.6583
3	-2	2.8139	4.2500	-1.4361
3.5	-1.5	3.2753	4.5000	-1.2247
4	-1	3.7192	4.7500	-1.0308
4.5	-0.5	4.1340	5.0000	-0.8660
4.75	-0.25	4.3246	5.1250	-0.8004
4.95	-0.05	4.4663	5.2250	-0.7587
5	0	4.5000	5.2500	-0.7500
5.05	0.05	4.5330	5.2750	-0.7420
5.25	0.25	4.6569	5.3750	-0.7181
5.5	0.5	4.7929	5.5000	-0.7071
6	1	5.0000	5.7500	-0.7500
6.5	1.5	5.1340	6.0000	-0.8660
7	2	5.2192	6.2500	-1.0308
7.5	2.5	5.2753	6.5000	-1.2247

Table S3. Values of T_1 and T_2 for the state with energy E_3 (case 2a).

α_1 (eV)	ε (eV)	E_3 (eV)	T_1 (eV)	T_2 (eV)
2.5	-2.5	5.6583	4.0000	1.6583
3	-2	5.6861	4.2500	1.4361
3.5	-1.5	5.7247	4.5000	1.2247
4	-1	5.7808	4.7500	1.0308
4.5	-0.5	5.8660	5.0000	0.8660
4.75	-0.25	5.9254	5.1250	0.8004
4.95	-0.05	5.9837	5.2250	0.7587
5	0	6.0000	5.2500	0.7500
5.05	0.05	6.0170	5.2750	0.7420
5.25	0.25	6.0931	5.3750	0.7181
5.5	0.5	6.2071	5.5000	0.7071
6	1	6.5000	5.7500	0.7500
6.5	1.5	6.8660	6.0000	0.8660
7	2	7.2808	6.2500	1.0308
7.5	2.5	7.7247	6.5000	1.2247

For values of α_1 smaller than 5.5 eV ($\varepsilon < \beta$), ε contributes mainly to the energy of the E_2 state. When α_1 becomes larger than 5.5 eV ($\varepsilon > \beta$), E_3 takes advantage of the increasing ε value to raise its energy. The oscillator strength S_2 of E_2 grows as the value of α_1 changes from the 5 eV resonance value where $\alpha_1 = \alpha_2 = \alpha_3$ (the ideal case 1). On the other hand, the oscillator strength S_3 of the plasmon peak reaches a maximum for this value of α_1. S_3 therefore "borrows" less oscillator strength from S_2 when $\alpha_1 \neq \alpha$. We note that S_3 always has a larger value than S_2 in the α_1 range considered. The eigenvectors of all the matrices studied are reported in Tables S4-S17. The coefficients A_i contributing to the plasmon peak (with energy E_3) all have the same sign. The constructive interaction of the individual transitions making the plasmon therefore remains. We see that for E_1, $A_1 = 0$, $A_2 = 1/\sqrt{2}$ and $A_3 = -1/\sqrt{2}$ regardless of the value of α_1. This reflects that only transitions 2 and 3 contribute to that peak and their contributions remain constant. This is not surprising since $\alpha_2 = \alpha_3 = 5$ eV and all coupling constants are equal for all values of α_1. For E_2 and E_3, the contributions of transitions 2 and 3 are identical regardless of the value of α_1 ($A_2 = A_3$). As α_1 becomes larger, the contributions of transitions 2 and 3 increase for E_2 and decrease for E_3. On the other hand, $|A_1|$ increases for E_3 and decreases for E_2. This shows the growing contribution of transition 1 to E_3 as α_1 becomes larger. For $\alpha_1 >> \alpha$, it would be reasonable to expect that only transition one will contribute to the peak at energy E_3. E_3 will then be labeled as a single-electron transition and no longer be a plasmon. Only transitions two and three will mix efficiently and a high-intensity plasmon peak at 5.5 eV will result from the constructive interaction of these two transitions. Another peak with zero oscillator strength will occur at 4.5 eV. This illustrates why the configurations in the CI must be close in energy to create a plasmon. Overall, changing one of the values of α not only lifts the degeneracy between E_1 and E_2, but it also increases the oscillator strength of the peak at energy E_2, which would make it observable in

the absorption spectrum. The increase in oscillator strength for E_2 also leads to a decrease in oscillator strength for the state at energy E_3, which is the plasmon.

Table S4. Eigenvectors of the CI matrix for case 2a where α_1=2.5 eV.

	E_1= 4.5 eV	E_2= 2.3417 eV	E_3= 5.6583 eV
A_1	0	0.9758	0.2185
A_2	0.7071	-0.1545	0.6900
A_3	-0.7071	-0.1545	0.6900
$\|A_1+A_2+A_3\|^2$	0	0.4448	2.5552

Table S5. Eigenvectors of the CI matrix for case 2a where α_1=3.0 eV.

	E_1= 4.5 eV	E_2= 2.8139 eV	E_3= 5.6861 eV
A_1	0	0.9671	0.2546
A_2	0.7071	-0.1800	0.6838
A_3	-0.7071	-0.1800	0.6838
$\|A_1+A_2+A_3\|^2$	0	0.3684	2.6315

Table S6. Eigenvectors of the CI matrix for case 2a where α_1=3.5 eV.

	E_1= 4.5 eV	E_2= 3.2753 eV	E_3= 5.7247 eV
A_1	0	0.9530	0.3029
A_2	0.7071	-0.2142	0.6739
A_3	-0.7071	-0.2142	0.6739
$\|A_1+A_2+A_3\|^2$	0	0.2752	2.7248

Table S7. Eigenvectors of the CI matrix for case 2a where α_1=4.0 eV.

	E_1= 4.5 eV	E_2= 3.7192 eV	E_3= 5.7808 eV
A_1	0	0.9294	0.3690
A_2	0.7071	-0.2610	0.6572
A_3	-0.7071	-0.2610	0.6572
$\|A_1+A_2+A_3\|^2$	0	0.1661	2.8338

Table S8. Eigenvectors of the CI matrix for case 2a where α_1=4.5 eV.

	E_1= 4.5 eV	E_2= 4.1340 eV	E_3= 5.8660 eV
A_1	0	0.8881	0.4597
A_2	0.7071	-0.3251	0.6280
A_3	-0.7071	-0.3251	0.6280
$\|A_1+A_2+A_3\|^2$	0	0.0.0566	2.9432

Table S9. Eigenvectors of the CI matrix for case 2a where α_1=4.75 eV.

	E_1= 4.5 eV	E_2= 4.3246 eV	E_3= 5.9254 eV
A_1	0	0.8569	0.5155
A_2	0.7071	-0.3645	0.6059
A_3	-0.7071	-0.3645	0.6059
$\|A_1+A_2+A_3\|^2$	0	0.0164	2.9836

Table S10. Eigenvectors of the CI matrix for case 2a where α_1=4.95 eV.

	E_1= 4.5 eV	E_2= 4.4663 eV	E_3= 5.9837 eV
A_1	0	0.8254	0.5646
A_2	0.7071	-0.3992	0.5836
A_3	-0.7071	-0.3992	0.5836
$\|A_1+A_2+A_3\|^2$	0	0.0007	2.9991

Table S11. Eigenvectors of the CI matrix for case 2a where α_1=5.05 eV.

	E_1= 4.5 eV	E_2= 4.533 eV	E_3= 6.017 eV
A_1	0	0.8072	0.5902
A_2	0.7071	-0.4174	0.5708
A_3	-0.7071	-0.4174	0.5708
$\|A_1+A_2+A_3\|^2$	0	0.0008	2.9991

Table S12. Eigenvectors of the CI matrix for case 2a where α_1=5.25 eV.

	E_1= 4.5 eV	E_2= 4.6569 eV	E_3= 6.0931 eV
A_1	0	0.7662	0.6426
A_2	0.7071	-0.4544	0.5418
A_3	-0.7071	-0.4544	0.5418
$\|A_1+A_2+A_3\|^2$	0	0.0203	2.9798

Table S13. Eigenvectors of the CI matrix for case 2a where α_1=5.5 eV.

	E_1= 4.5 eV	E_2= 4.7929 eV	E_3= 6.2071 eV
A_1	0	0.7071	0.7071
A_2	0.7071	-0.5	0.5
A_3	-0.7071	-0.5	0.5
$\|A_1+A_2+A_3\|^2$	0	0.0858	2.9142

Table S14. Eigenvectors of the CI matrix for case 2a where α_1=6.0 eV.

	E_1= 4.5 eV	E_2= 5.0 eV	E_3= 6.5 eV
A_1	0	0.5774	0.8165
A_2	0.7071	-0.5774	0.4082
A_3	-0.7071	-0.5774	0.4082
$\|A_1+A_2+A_3\|^2$	0	0.3334	2.6663

Table S15. Eigenvectors of the CI matrix for case 2a where α_1=6.5 eV.

	E_1= 4.5 eV	E_2= 5.134 eV	E_3= 6.866 eV
A_1	0	0.4597	-0.8881
A_2	0.7071	-0.628	-0.3251
A_3	-0.7071	-0.628	-0.3251
$\|A_1+A_2+A_3\|^2$	0	0.6341	2.3664

Table S16. Eigenvectors of the CI matrix for case 2a where α_1=7 eV.

	E_1= 4.5 eV	E_2= 5.2192 eV	E_3= 7.2808 eV
A_1	0	0.369	-0.9294
A_2	0.7071	-0.6572	-0.261
A_3	-0.7071	-0.6572	-0.261
$\|A_1+A_2+A_3\|^2$	0	0.8938	2.1066

Table S17. Eigenvectors of the CI matrix for case 2a where α_1=7.5 eV.

	E_1= 4.5 eV	E_2= 5.2753 eV	E_3= 7.7247 eV
A_1	0	0.3029	-0.953
A_2	0.7071	-0.6739	-0.2142
A_3	-0.7071	-0.6739	-0.2142
$\|A_1+A_2+A_3\|^2$	0	1.0918	1.9083

Case 2: Allow all three α values to differ

Table S18. Energies and oscillator strengths for different values of α_3 (case 2).

$\Delta\alpha_3$(%)	α_3 (eV)	E_1 (eV)	S_1 (a.u)	E_2 (eV)	S_2 (a.u.)	E_3 (eV)	S_3 (a.u.)
-50	2.5	2.359	0.4952	4.8207	0.3329	6.3202	2.1718
-40	3	2.836	0.4273	4.8272	0.3408	6.3368	2.2317
-30	3.5	3.3038	0.3407	4.8373	0.3520	6.3589	2.3074
-20	4	3.7554	0.2290	4.8554	0.3681	6.3892	2.4028
-10	4.5	4.1723	0.0918	4.8946	0.3846	6.4331	2.5236
-5	4.75	4.3532	0.0284	4.9339	0.3785	6.4628	2.5931
-1	4.95	4.4741	0.0012	4.9841	0.3469	6.4919	2.6517
0	5.0	4.5	0.0000	5.0	0.3334	6.5	2.6664
1	5.05	4.5241	0.0012	5.0174	0.3173	6.5085	2.6814
5	5.25	4.6015	0.0279	5.1014	0.2331	6.5471	2.7390
10	5.5	4.6624	0.0832	5.2304	0.1160	6.6072	2.8009
20	6	4.7192	0.1661	5.5	0.0000	6.7808	2.8338
30	6.5	4.7429	0.2070	5.714	0.1151	7.0431	2.6778
50	7.5	4.7629	0.2290	5.9437	0.3681	7.7934	2.4028

Table S19. Eigenvectors of the CI matrix for case 2 where α_3=2.5 eV.

	E_1= 2.3590 eV	E_2= 4.8207 eV	E_3= 6.3202 eV
A_1	-0.1120	-0.4248	-0.8983
A_2	-0.1643	0.8995	-0.4048
A_3	0.9800	0.1023	-0.1706
$\|A_1+A_2+A_3\|^2$	0.4952	0. 3329	2.1718

Table S20. Eigenvectors of the CI matrix for case 2 where α_3=3.0 eV.

	E_1= 2.8360 eV	E_2= 4.8272 eV	E_3= 6.3368 eV
A_1	-0.1227	-0.4338	-0.8926
A_2	-0.1964	0.8922	-0.4067
A_3	0.9728	0.1254	-0.1947
$\|A_1+A_2+A_3\|^2$	0.4273	0.3408	2.2317

Table S21. Eigenvectors of the CI matrix for case 2 where α_3=3.5 eV.

	E_1= 3.3038 eV	E_2= 4.8373 eV	E_3= 6.3589 eV
A_1	-0.1329	-0.4477	-0.8843
A_2	-0.2440	0.8795	-0.4086
A_3	0.9606	0.1615	-0.2261
$\|A_1+A_2+A_3\|^2$	0.3407	0.3520	2.3074

Table S22. Eigenvectors of the CI matrix for case 2 where α_3=4.0 eV.

	E_1= 3.7554 eV	E_2= 4.8554 eV	E_3= 6.3892 eV
A_1	-0.1371	-0.4706	-0.8716
A_2	-0.3213	0.8535	-0.4103
A_3	0.9370	0.2238	-0.2683
$\|A_1+A_2+A_3\|^2$	0.2290	0.3681	2.4028

Table S23. Eigenvectors of the CI matrix for case 2 where α_3=4.5 eV.

	E_1= 4.1723 eV	E_2= 4.8946 eV	E_3= 6.4331eV
A_1	-0.1141	-0.5122	-0.8512
A_2	-0.4623	0.7858	-0.4109
A_3	0.8794	0.3466	-0.3265
$\|A_1+A_2+A_3\|^2$	0.0918	0.3846	2.5237

Table S24. Eigenvectors of the CI matrix for case 2 where α_3=4.75 eV.

	E_1= 4.3532 eV	E_2= 4.9339 eV	E_3= 6.4628eV
A_1	-0.0734	-0.5434	-0.8363
A_2	-0.5738	0.7088	-0.4102
A_3	0.8157	0.4497	-0.3639
$\|A_1+A_2+A_3\|^2$	0.0284	0.3785	2.5931

Table S25. Eigenvectors of the CI matrix for case 2 where α_3=4.95 eV.

	E_1= 4.4741 eV	E_2= 4.9841 eV	E_3= 6.4919 eV
A_1	0.0172	0.5708	-0.8209
A_2	0.6803	-0.6084	-0.4088
A_3	-0.7328	-0.5514	-0.3988
$\|A_1+A_2+A_3\|^2$	0.0012	0.3469	2.6517

Table S26. Eigenvectors of the CI matrix for case 2 where α_3=5.05 eV.

	E_1= 4.5241 eV	E_2= 5.0174 eV	E_3= 6.5085 eV
A_1	-0.0181	0.5836	0.8118
A_2	0.7332	-0.5443	0.4076
A_3	-0.6798	-0.6026	0.4180
$\|A_1+A_2+A_3\|^2$	0.0012	0.3173	2.6814

Table S27. Eigenvectors of the CI matrix for case 2 where α_3=5.25 eV.

	E_1= 4.6015 eV	E_2= 5.1014 eV	E_3= 6.5471 eV
A_1	-0.0929	-0.6056	0.7903
A_2	0.8219	0.4014	0.4042
A_3	-0.5621	0.6870	0.4605
$\|A_1+A_2+A_3\|^2$	0.0279	0.2331	2.7390

Table S28. Eigenvectors of the CI matrix for case 2 where α_3=5.5 eV.

	E_1= 4.6624 eV	E_2= 5.2304 eV	E_3= 6.6072 eV
A_1	-0.1721	-0.6318	0.7558
A_2	0.8877	0.2332	0.3971
A_3	-0.4271	0.7392	0.5207
$\|A_1+A_2+A_3\|^2$	0.0832	0.1160	2.8009

Table S29. Eigenvectors of the CI matrix for case 2 where α_3=6.0 eV.

	E_1= 4.7192 eV	E_2= 5.50 eV	E_3= 6.7808 eV
A_1	0.2610	0.7071	0.6572
A_2	-0.9294	0	0.3690
A_3	0.2610	-0.7071	0.6572
$\|A_1+A_2+A_3\|^2$	0.1917	0	2.8338

Table S30. Eigenvectors of the CI matrix for case 2 where α_3=6.5 eV.

	E_1= 4.7429 eV	E_2= 5.7140 eV	E_3= 7.0431 eV
A_1	0.3005	0.7928	-0.5302
A_2	-0.9365	0.1398	0.3217
A_3	0.1810	-0.5932	0.7844
$\|A_1+A_2+A_3\|^2$	0.2070	0.1151	2.6778

Table S31. Eigenvectors of the CI matrix for case 2 where α_3=7 eV.

	E_1= 4.7554 eV	E_2= 5.8554 eV	E_3= 7.3892 eV
A_1	0.3213	0.8535	0.4103
A_2	-0.9370	0.2238	0.2683
A_3	-0.1371	-0.4706	0.8716
$\|A_1+A_2+A_3\|^2$	0.2290	0.3681	2.4028

Table S32. Eigenvectors of the CI matrix for case 2 where α_3=7.5 eV.

	E_1= 4.7629 eV	E_2= 5.9437 eV	E_3= 7.7934 eV
A_1	0.3339	0.8871	0.3188
A_2	-0.9362	0.2726	0.2220
A_3	0.1100	-0.3726	0.9215
$\|A_1+A_2+A_3\|^2$	0.2423	0.6195	2.1380

Case 3a: Vary β_{12} only

We here investigate how changing the coupling values β affects the absorption spectrum of the system. Only the coupling between transitions 1 and 2 is changed. The CI matrix studied in this section is:

$$\begin{bmatrix} 5 & \beta_{12} & 0.5 \\ \beta_{12} & 5 & 0.5 \\ 0.5 & 0.5 & 5 \end{bmatrix} \quad (3)$$

The values of β_{12} considered are varied by ±1, ±5, ±10, ±20, ±30, ±40 and ±50% of the value used in case 1 (0.5 eV), which gives β_{12}= 0.25, 0.30, 0.35, 0.40, 0.45, 0.475, 0.495, 0.505, 0.525, 0.55, 0.60, 0.65, 0.70 and 0.75 eV. The peak energies and oscillator strengths are reported in

Figure S2 and in Table S33. The eigenvectors for each matrix studied in this section are reported in Tables S34 to S47.

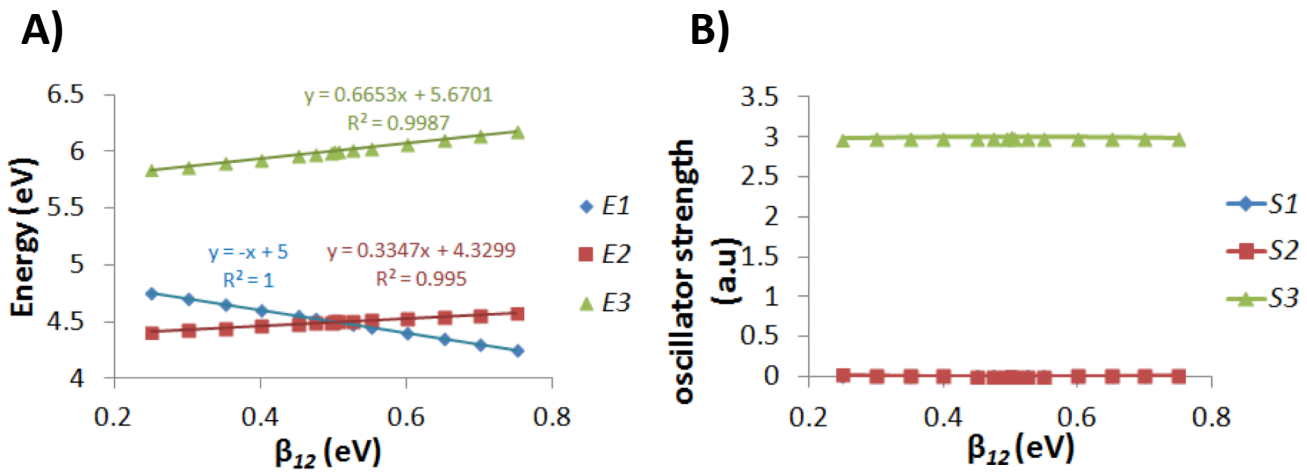

Figure S2. A) Peak energies and B) oscillator strengths for different values of β_{12} (case 4).

State E_3 has the highest energy as well as the highest oscillator strength due to a constructive addition of its eigenvectors. Like in the previous cases, this state is the plasmon. One of the three excited states has $A_1 = -A_2 = 1/\sqrt{2}$ and A_3= 0 for all values of β_{12} (except in the ideal case where β_{12}=0.5 eV, due to the normalization of the eigenvectors). This state is labeled with energy E_1 and it has zero oscillator strength. It crosses with E_2 at β_{12}= 0.5 eV. The amplitude of the variation of the peak energies is very small (less than 0.5 eV), due to the fact that the values of β considered are only approximately 10% of the values of α. We can see that the energies of states 2 and 3 increase linearly with increasing β_{12} whereas the energy of state 1 decreases linearly. E_2 and E_3 use the intensifying coupling between transitions 1 and 2 to increase their energy, which results in a decrease of E_1. The decrease in E_1 (indicated by the opposite value of the slope of the linear fit of E_1 as a function of β_{12}) is equal to the increase of

E_2 plus the increase of E_3. The oscillator strengths of the three excited states are nearly identical to those obtained for the ideal case regardless of the value of β_{12}. The plasmon state oscillator strength grows as β_{12} approaches the 0.5 eV value of the ideal case. However, the change is so small that the oscillator strength appears constant. The oscillator strength of state 2 slightly increases as the value of β_{12} differs more from the original 0.5 eV value but it remains so small that it is essentially 0. We can also see that $A_1 = A_2$ for the eigenvalues E_2 and E_3 regardless of the β_{12} value, reflecting the identical contributions of transitions 1 and 2. As β_{12} increases, we see that $|A_1|$ and $|A_2|$ decrease whereas $|A_3|$ increases for E_2 and vice versa for E_3.

Table S33. Energies and oscillator strengths for varying values of β_{12} (case 3a).

$\Delta\beta_{12}$(%)	β_{12} (eV)	E_1 (eV)	S_1 (a.u.)	E_2 (eV)	S_2 (a.u.)	E_3 (eV)	S_3 (a.u.)
-50	0.25	4.75	0	4.4069	0.0203	5.8431	2.9798
-40	0.3	4.7	0	4.4272	0.0128	5.8728	2.9870
-30	0.35	4.65	0	4.4466	0.0071	5.9034	2.9929
-20	0.4	4.6	0	4.4652	0.0031	5.9348	2.9971
-10	0.45	4.55	0	4.483	0.0008	5.967	2.9991
-5	0.475	4.525	0	4.4916	0.0002	5.9834	2.9998
-1	0.495	4.505	0	4.4983	$7.29*10^{-6}$	5.9967	2.9998
0	0.5	4.5	0	4.5	0.0000	6	3.0005
1	0.505	4.495	0	4.5017	$7.84*10^{-6}$	6.0033	3.0002
5	0.525	4.475	0	4.5082	0.0002	6.0168	2.9998
10	0.55	4.45	0	4.5163	0.0007	6.0337	2.9991
20	0.6	4.4	0	4.5319	0.0028	6.0681	2.9971
30	0.65	4.35	0	4.5468	0.0062	6.1032	2.9936
40	0.7	4.3	0	4.561	0.0107	6.139	2.9894
50	0.75	4.25	0	4.5746	0.0164	6.1754	2.9836

Table S34. Eigenvectors of the CI matrix for case 3a where β_{12}=0.25 eV.

	E_1= 4.75 eV	E_2= 4.4069 eV	E_3= 5.8431 eV
A_1	0.7071	0.4544	0.5418
A_2	-0.7071	0.4544	0.5418
A_3	0	-0.7662	0.6426
$\|A_1+A_2+A_3\|^2$	0	0.0203	2.9798

Table S35. Eigenvectors of the CI matrix for case 3a where β_{12}=0.3 eV.

	E_1= 4.70 eV	E_2= 4.4272 eV	E_3= 5.8728 eV
A_1	0.7071	0.4451	0.5494
A_2	-0.7071	0.4451	0.5494
A_3	0	-0.7770	0.6295
$\|A_1+A_2+A_3\|^2$	0	0.0128	2.9870

Table S36. Eigenvectors of the CI matrix for case 3a where β_{12}=0.35 eV.

	E_1= 4.65 eV	E_2= 4.4466 eV	E_3= 5.9034 eV
A_1	0.7071	0.4358	0.5568
A_2	-0.7071	0.4358	0.5568
A_3	0	-0.7875	0.6163
$\|A_1+A_2+A_3\|^2$	0	0.0071	2.9929

Table S37. Eigenvectors of the CI matrix for case 3a where β_{12}=0.40 eV.

	E_1= 4.60 eV	E_2= 4.4652 eV	E_3= 5.9348 eV
A_1	0.7071	0.4266	0.5640
A_2	-0.7071	0.4266	0.5640
A_3	0	-0.7975	0.6033
$\|A_1+A_2+A_3\|^2$	0	0.0031	2.9971

Table S38. Eigenvectors of the CI matrix for case 3a where β_{12}=0.45 eV.

	E_1= 4.55 eV	E_2= 4.483 eV	E_3= 5.967 eV
A_1	0.7071	0.4174	0.5708
A_2	-0.7071	0.4174	0.5708
A_3	0	-0.8072	0.5902
$\|A_1+A_2+A_3\|^2$	0	0.0008	2.9991

Table S39. Eigenvectors of the CI matrix for case 3a where β_{12}=0.475 eV.

	E_1= 4.5250 eV	E_2= 4.4916 eV	E_3= 5.9834 eV
A_1	0.7071	0.4128	0.5741
A_2	-0.7071	0.4128	0.5741
A_3	0	-0.8119	0.5838
$\|A_1+A_2+A_3\|^2$	0	0.0002	2.9998

Table S40. Eigenvectors of the CI matrix for case 3a where β_{12}=0.495 eV.

	E_1= 4.5050 eV	E_2= 4.4983 eV	E_3= 5.9967 eV
A_1	0.7071	0.4092	0.5767
A_2	-0.7071	0.4092	0.5767
A_3	0	-0.8156	0.5786
$\|A_1+A_2+A_3\|^2$	0	$7.29*10^{-6}$	2.9998

Table S41. Eigenvectors of the CI matrix for case 3a where β_{12}=0.505 eV.

	E_1= 4.495 eV	E_2= 4.5017 eV	E_3= 6.0033 eV
A_1	0.7071	0.4073	0.578
A_2	-0.7071	0.4073	0.578
A_3	0	-0.8174	0.5761
$\|A_1+A_2+A_3\|^2$	0	$7.84*10^{-6}$	3.000

Table S42. Eigenvectors of the CI matrix for case 3a where β_{12}=0.525 eV.

	E_1= 4.475 eV	E_2= 4.5082 eV	E_3= 6.0168 eV
A_1	0.7071	0.4037	0.5805
A_2	-0.7071	0.4037	0.5805
A_3	0	-0.821	0.571
$\|A_1+A_2+A_3\|^2$	0	0.0002	2.9998

Table S43. Eigenvectors of the CI matrix for case 3a where β_{12}=0.55 eV.

	E_1= 4.45 eV	E_2= 4.5163 eV	E_3= 6.0337 eV
A_1	0.7071	0.3992	0.5836
A_2	-0.7071	0.3992	0.5836
A_3	0	-0.8254	0.5646
$\|A_1+A_2+A_3\|^2$	0	0.0007	2.9991

Table S44. Eigenvectors of the CI matrix for case 3a where β_{12}=0.60 eV.

	E_1= 4.40 eV	E_2= 4.5319 eV	E_3= 6.0681 eV
A_1	0.7071	0.3903	0.5896
A_2	-0.7071	0.3903	0.5896
A_3	0	-0.8338	0.5520
$\|A_1+A_2+A_3\|^2$	0	0.0028	2.9971

Table S45. Eigenvectors of the CI matrix for case 3a where β_{12}=0.65 eV.

	E_1= 4.35 eV	E_2= 4.5468 eV	E_3= 6.1032 eV
A_1	0.7071	0.3816	0.5953
A_2	-0.7071	0.3816	0.5953
A_3	0	-0.8419	0.5396
$\|A_1+A_2+A_3\|^2$	0	0.0062	2.9939

Table S46. Eigenvectors of the CI matrix for case 3a where β_{12}=0.70 eV.

	E_1= 4.30 eV	E_2= 4.5610 eV	E_3= 6.1390 eV
A_1	0.7071	0.3730	0.6008
A_2	-0.7071	0.3730	0.6008
A_3	0	-0.8496	0.5274
$\|A_1+A_2+A_3\|^2$	0	0.0108	2.9891

Table S47. Eigenvectors of the CI matrix for case 3a where β_{12}=0.75 eV.

	E_1= 4.25 eV	E_2= 4.5746 eV	E_3= 6.1754 eV
A_1	0.7071	0.3645	0.6059
A_2	-0.7071	0.3645	0.6059
A_3	0	-0.8569	0.5155
$\|A_1+A_2+A_3\|^2$	0	0.0164	2.9836

Case 3: Vary β_{12} and β_{23}

Table S48. Energies and oscillator strengths for varying values of β_{23} (case 3).

$\Delta\beta_{23}$(%)	β_{23} (eV)	E_1 (eV)	S_1 (a.u.)	E_2 (eV)	S_2 (a.u.)	E_3 (eV)	S_3 (a.u.)
-50	0.25	4.3303	0.0220	4.7551	0.0077	5.9146	2.9705
-40	0.3	4.3493	0.0144	4.7069	0.0067	5.9438	2.9787
-30	0.35	4.3669	0.0084	4.6593	0.0059	5.9737	2.9856
-20	0.4	4.3825	0.0039	4.6131	0.0051	6.0045	2.9912
-10	0.45	4.3946	0.0010	4.5695	0.0042	6.0359	2.9950
-5	0.475	4.3985	0.0003	4.5496	0.0036	6.0519	2.9960
-1	0.495	4.3999	0.00001	4.5352	0.0030	6.0649	2.9971
0	0.5	4.4	0.0000	4.5319	0.0028	6.0681	2.9971
1	0.505	4.3999	0.00001	4.5287	0.0027	6.0714	2.9974
5	0.525	4.3981	0.0002	4.5174	0.0019	6.0845	2.9977
10	0.55	4.3918	0.0009	4.5072	0.0010	6.101	2.9981
20	0.6	4.3654	0.0021	4.5	0.0000	6.1346	2.9977
30	0.65	4.3268	0.0027	4.5043	0.0009	6.1688	2.9964
40	0.7	4.2828	0.0028	4.5135	0.0035	6.2037	2.9939
50	0.75	4.2363	0.0027	4.5245	0.0071	6.2392	2.9901

Table S49. Eigenvectors of the CI matrix for case 3 where β_{23}=0.25 eV.

	E_1= 4.3303 eV	E_2= 4.7551 eV	E_3= 5.9146 eV
A_1	0.7573	0.0717	0.6491
A_2	-0.5431	0.6211	0.5650
A_3	-0.3627	-0.7804	0.5093
$\|A_1+A_2+A_3\|^2$	0.0220	0.0077	2.9705

Table S50. Eigenvectors of the CI matrix for case 3 where β_{23}=0.30 eV.

	E_1= 4.3493 eV	E_2= 4.7069 eV	E_3= 5.9438 eV
A_1	0.7647	0.0960	0.6372
A_2	-0.5515	0.6091	0.5700
A_3	-0.3334	-0.7872	0.5188
$\|A_1+A_2+A_3\|^2$	0.0144	0.0067	2.9787

Table S51. Eigenvectors of the CI matrix for case 3 where β_{23}=0.35 eV.

	E_1= 4.3669 eV	E_2= 4.6593 eV	E_3= 5.9737 eV
A_1	0.7696	0.1296	0.6253
A_2	-0.5665	0.5903	0.5750
A_3	-0.2946	-0.7967	0.5277
$\|A_1+A_2+A_3\|^2$	0.0084	0.0059	2.9856

Table S52. Eigenvectors of the CI matrix for case 3 where β_{23}=0.40 eV.

	E_1= 4.3825 eV	E_2= 4.6131 eV	E_3= 6.0045 eV
A_1	0.7692	0.1792	0.6133
A_2	-0.5926	0.5591	0.5799
A_3	-0.2390	-0.8095	0.5362
$\|A_1+A_2+A_3\|^2$	0.0039	0.0051	2.9912

Table S53. Eigenvectors of the CI matrix for case 3 where β_{23}=0.45 eV.

	E_1= 4.3946 eV	E_2= 4.5695 eV	E_3= 6.0359 eV
A_1	0.7559	0.2598	0.6014
A_2	-0.6371	0.5021	0.5848
A_3	-0.1507	-0.8252	0.5443
$\|A_1+A_2+A_3\|^2$	0.0010	0.0042	2.9950

Table S54. Eigenvectors of the CI matrix for case 3 where β_{23}=0.475 eV.

	E_1= 4.3985 eV	E_2= 4.5496 eV	E_3= 6.0519 eV
A_1	0.7383	0.3166	0.5955
A_2	-0.6690	0.4556	0.5872
A_3	-0.0854	-0.8320	0.5482
$\|A_1+A_2+A_3\|^2$	0.0003	0.0036	2.9960

Table S55. Eigenvectors of the CI matrix for case 3 where β_{23}=0.495 eV.

	E_1= 4.3999 eV	E_2= 4.5352 eV	E_3= 6.0649 eV
A_1	0.7147	0.3743	0.5908
A_2	-0.6991	0.4051	0.5891
A_3	-0.0188	-0.8341	0.5513
$\|A_1+A_2+A_3\|^2$	0.00001	0.0030	2.9971

Table S56. Eigenvectors of the CI matrix for case 3 where β_{23}=0.505 eV.

	E_1= 4.3999 eV	E_2= 4.5287 eV	E_3= 6.0714 eV
A_1	0.6987	0.4070	0.5884
A_2	-0.7152	0.3746	0.5901
A_3	-0.0197	-0.8331	0.5528
$\|A_1+A_2+A_3\|^2$	0.00001	0.0027	2.9974

Table S57. Eigenvectors of the CI matrix for case 3 where β_{23}=0.525 eV.

	E_1= 4.3981 eV	E_2= 4.5174 eV	E_3= 6.0845 eV
A_1	0.6562	0.4781	0.5837
A_2	-0.7470	0.3026	0.5920
A_3	0.1064	-0.8245	0.5557
$\|A_1+A_2+A_3\|^2$	0.0002	0.0019	2.9977

Table S58. Eigenvectors of the CI matrix for case 3 where β_{23}=0.55 eV.

	E_1= 4.3918 eV	E_2= 4.5072 eV	E_3= 6.1010 eV
A_1	0.5846	0.5695	0.5779
A_2	-0.7797	0.1973	0.5943
A_3	0.2244	-0.7980	0.5593
$\|A_1+A_2+A_3\|^2$	0.009	0.0010	2.9981

Table S59. Eigenvectors of the CI matrix for case 3 where β_{23}=0.60 eV.

	E_1= 4.3654 eV	E_2= 4.5000 eV	E_3= 6.1346 eV
A_1	-0.4235	-0.7071	0.5663
A_2	0.8008	0	0.5989
A_3	-0.4235	0.7071	0.5663
$\|A_1+A_2+A_3\|^2$	0.0021	0	2.9977

Table S60. Eigenvectors of the CI matrix for case 3 where β_{23}=0.65 eV.

	E_1= 4.3268 eV	E_2= 4.5043 eV	E_3= 6.1688 eV
A_1	-0.3061	-0.7736	0.5548
A_2	0.7883	0.1207	0.6034
A_3	-0.5338	0.6220	0.5729
$\|A_1+A_2+A_3\|^2$	0.0027	0.0009	2.9964

Table S61. Eigenvectors of the CI matrix for case 3 where β_{23}=0.70 eV.

	E_1= 4.2828 eV	E_2= 4.5135 eV	E_3= 6.2037 eV
A_1	-0.2347	0.8060	0.5435
A_2	0.7724	-0.1849	0.6077
A_3	-0.5902	-0.5624	0.5791
$\|A_1+A_2+A_3\|^2$	0.0028	0.0035	2.9939

Table S62. Eigenvectors of the CI matrix for case 3 where β_{23}=0.75 eV.

	E_1= 4.2363 eV	E_2= 4.5245 eV	E_3= 6.2392 eV
A_1	-0.1898	0.8250	0.5323
A_2	0.7598	-0.2200	0.6118
A_3	-0.6219	-0.5205	0.5851
$\|A_1+A_2+A_3\|^2$	0.0027	0.0071	2.9901

Case 4: Varying the β/α ratio

Table S63. Energies and oscillator strengths for varying values of β (case 4).

β (eV)	E_1 (eV)	S_1 (a.u.)	E_2 (eV)	S_2 (a.u.)	E_3 (eV)	S_3 (a.u.)
0	5.0000	1.0000	5.1000	1.0000	5.2000	1.0000
0.001	5.0000	0.9704	5.1000	0.9994	5.2000	1.0300
0.005	4.9996	0.8578	5.1000	0.9853	5.2004	1.1569
0.01	4.9986	0.7331	5.0998	0.9426	5.2016	1.3241
0.05	4.9755	0.2291	5.0855	0.3681	5.2389	2.4031
0.1	4.9325	0.0832	5.0461	0.1160	5.3214	2.8009
0.2	4.8370	0.0245	4.9520	0.0295	5.5110	2.9460
0.3	4.7387	0.0114	4.8539	0.0130	5.7074	2.9756
0.4	4.6396	0.0066	4.7549	0.0072	5.9055	2.9863
0.5	4.5401	0.0043	4.6555	0.0046	6.1044	2.9912
1	4.0412	0.0011	4.1566	0.0011	7.1022	2.9977
2	3.0417	0.0003	3.1572	0.0003	9.1011	2.9995

Table S64. Eigenvectors of the CI matrix for case 4 where β=0.

	E_1= 5.0000 eV	E_2= 5.1000 eV	E_3= 5.2000 eV
A_1	1	0	0
A_2	0	1	0
A_3	0	0	1
$\|A_1+A_2+A_3\|^2$	1	1	1

Table S65. Eigenvectors of the CI matrix for case 4 where β=0.001 eV.

	E_1= 5.0000 eV	E_2= 5.1000 eV	E_3= 5.2000 eV
A_1	0.9999	0.0099	0.005
A_2	-0.0099	0.9999	0.01
A_3	-0.0049	-0.0101	0.9999
$\|A_1+A_2+A_3\|^2$	0.9704	0.9994	1.0300

Table S66. Eigenvectors of the CI matrix for case 4 where β=0.005 eV.

	E_1= 4.9996 eV	E_2= 5.1000 eV	E_3= 5.2004 eV
A_1	0.9985	0.0473	0.0262
A_2	-0.0486	0.9975	0.051
A_3	-0.0237	-0.0522	0.9984
$\|A_1+A_2+A_3\|^2$	0.8579	0.9853	1.1569

Table S67. Eigenvectors of the CI matrix for case 4 where β=0.01 eV.

	E_1= 4.9986 eV	E_2= 5.0998 eV	E_3= 5.2016 eV
A_1	0.9946	0.0884	0.0544
A_2	-0.0937	0.9902	0.1031
A_3	-0.0447	-0.1077	0.9932
$\|A_1+A_2+A_3\|^2$	0.733078	0.942647	1.32411

Table S68. Eigenvectors of the CI matrix for case 4 where β=0.05 eV.

	E_1= 4.9755 eV	E_2= 5.0855 eV	E_3= 5.2389 eV
A_1	0.937	0.2238	0.2683
A_2	-0.3213	0.8535	0.4103
A_3	-0.1371	-0.4706	0.8716
$\|A_1+A_2+A_3\|^2$	0.2291	0.3681	2.4031

Table S69. Eigenvectors of the CI matrix for case 4 where β=0.10 eV.

	E_1= 4.9325 eV	E_2= 5.0461 eV	E_3= 5.3214 eV
A_1	0.8877	0.2332	0.3971
A_2	-0.4271	0.7392	0.5207
A_3	-0.1721	-0.6318	0.7558
$\|A_1+A_2+A_3\|^2$	0.0832	0.1160	2.8009

Table S70. Eigenvectors of the CI matrix for case 4 where β=0.2 eV.

	E_1= 4.8370 eV	E_2= 4.9520 eV	E_3= 5.5110 eV
A_1	0.846	0.2261	0.4828
A_2	-0.4973	0.6611	0.5618
A_3	-0.1922	-0.7154	0.6718
$\|A_1+A_2+A_3\|^2$	0.0245	0.0295	2.9460

Table S71. Eigenvectors of the CI matrix for case 4 where β=0.3 eV.

	E_1= 4.7387 eV	E_2= 4.8539 eV	E_3= 5.7074 eV
A_1	0.8288	0.2219	0.5137
A_2	-0.5231	0.6333	0.5703
A_3	-0.1988	-0.7414	0.641
$\|A_1+A_2+A_3\|^2$	0.0114	0.0130	2.9756

Table S72. Eigenvectors of the CI matrix for case 4 where β=0.4 eV.

	E_1= 4.6396 eV	E_2= 4.7549 eV	E_3= 5.9055 eV
A_1	0.8195	0.2195	0.5295
A_2	-0.5364	0.6193	0.5734
A_3	-0.2021	-0.7538	0.6252
$\|A_1+A_2+A_3\|^2$	0.0066	0.0072	2.9863

Table S73. Eigenvectors of the CI matrix for case 4 where β=0.5 eV.

	E_1= 4.5401 eV	E_2= 4.6555 eV	E_3= 6.1044 eV
A_1	0.8136	0.218	0.539
A_2	-0.5444	0.6109	0.5748
A_3	-0.204	-0.7611	0.6157
$\|A_1+A_2+A_3\|^2$	0.0043	0.0046	2.9912

Table S74. Eigenvectors of the CI matrix for case 4 where β=1.0 eV.

	E_1= 4.0412 eV	E_2= 4.1566 eV	E_3= 7.1022 eV
A_1	0.8015	0.2148	0.5581
A_2	-0.5608	0.5941	0.5767
A_3	-0.2077	-0.7752	0.5966
$\|A_1+A_2+A_3\|^2$	0.0011	0.0011	2.9977

Table S75. Eigenvectors of the CI matrix for case 4 where β=2.0 eV.

	E_1= 3.0417 eV	E_2= 3.1572 eV	E_3= 9.1011 eV
A_1	0.7952	0.2131	0.5677
A_2	-0.569	0.5857	0.5772
A_3	-0.2095	-0.782	0.587
$\|A_1+A_2+A_3\|^2$	0.00028	0.00028	2.9995

Case 5: Mixed-coupling systems

Table S76. Eigenvectors of the CI matrix for case 5 where $\beta_{13}=\beta_{23}=0$

	E_1= 4.5475 eV	E_2= 5.2000 eV	E_3= 5.5525 eV
A_1	-0.7415	0	0.671
A_2	0.671	0	0.7415
A_3	0	1	0
$\lvert A_1+A_2+A_3\rvert^2$	0.0050	1	1.9952

Table S77. Eigenvectors of the CI matrix for case 5 where $\beta_{13}=\beta_{23}=0.001$ eV

	E_1= 4.5475 eV	E_2= 5.2000 eV	E_3= 5.5525 eV
A_1	0.7415	0.0026	0.671
A_2	-0.671	0.003	0.7414
A_3	-0.0001	-1	0.004
$\lvert A_1+A_2+A_3\rvert^2$	0.0050	0.9888	2.0062

Table S78. Eigenvectors of the CI matrix for case 5 where $\beta_{13}=\beta_{23}=0.005$ eV

	E_1= 4.5475 eV	E_2= 5.1999 eV	E_3= 5.5526 eV
A_1	0.7415	0.013	0.6709
A_2	-0.671	0.0152	0.7413
A_3	-0.0005	-0.9998	0.02
$\lvert A_1+A_2+A_3\rvert^2$	0.0049	0.9440	2.0512

Table S79. Eigenvectors of the CI matrix for case 5 where $\beta_{13}= \beta_{23}$=0.01 eV

	E_1= 4.5475 eV	E_2= 5.1994 eV	E_3= 5.5531 eV
A_1	0.7415	0.026	0.6705
A_2	-0.671	0.0304	0.7408
A_3	-0.0011	-0.9992	0.04
$\|A_1+A_2+A_3\|^2$	0.0048	0.8889	2.1062

Table S80. Eigenvectors of the CI matrix for case 5 where $\beta_{13}= \beta_{23}$=0.05 eV

	E_1= 4.5475 eV	E_2= 5.1864 eV	E_3= 5.5661 eV
A_1	0.7417	0.1231	0.6593
A_2	-0.6707	0.1441	0.7276
A_3	-0.0054	-0.9819	0.1894
$\|A_1+A_2+A_3\|^2$	0.0043	0.5108	2.4847

Table S81. Eigenvectors of the CI matrix for case 5 where $\beta_{13}= \beta_{23}$=0.1 eV

	E_1= 4.5474 eV	E_2= 5.1505 eV	E_3= 5.6021 eV
A_1	0.7425	0.2142	0.6347
A_2	-0.6698	0.2531	0.6981
A_3	-0.0111	-0.9434	0.3314
$\|A_1+A_2+A_3\|^2$	0.0038	0.2267	2.7696