Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reply to the 'Comment on "Elucidation of Charge-Transfer SERS Selection Rules by Considering the Excited State Properties and the Role of Electrode Potential"' by M. Mohammadpour, M. H. Khodabandeh, L. Visscher and Z. Jamshidi, Phys. Chem. Chem. Phys., 2017, 19, 7833

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Table S1. The calculated dimensionless displacements of 7 totally symmetric modes of Py-Ag_6 for 4 low-lying electronic state in different electric fields using the BP86 functional.

		External electric field (in au)						
State		**+0.0030**	**+0.0015**	**-0.0015**	**-0.0030**	**-0.0045**	**-0.0060**	**-0.0090**
S_1	ν_{6a}	1.0160	0.9845	0.9308	0.9063	0.8821	0.8587	0.8149
	ν_{1}	0.9040	0.9127	0.9331	0.9405	0.9493	0.9578	0.9740
	ν_{12}	0.3919	0.3660	0.3163	0.2933	0.2708	0.2496	0.2145
	ν_{19a}	0.1712	0.1810	0.1992	0.2069	0.2150	0.2230	0.2383
	ν_{9a}	0.9359	0.9273	0.9138	0.9078	0.9017	0.8960	0.8851
	ν_{18a}	0.1663	0.1598	0.1496	0.1456	0.1421	0.1394	0.1357
	ν_{8a}	0.9356	0.9293	0.9196	0.9151	0.9101	0.9053	0.8956
S_2	ν_{6a}	0.9766	0.9446	0.8899	0.8652	0.8409	0.8176	0.7744
	ν_{1}	0.8812	0.8890	0.9073	0.9140	0.9220	0.9296	0.9448
	ν_{12}	0.3756	0.3502	0.3011	0.2786	0.2565	0.2356	0.2012
	ν_{19a}	0.1507	0.1600	0.1772	0.1846	0.1924	0.2001	0.2150
	ν_{9a}	0.8896	0.8816	0.8691	0.8636	0.8580	0.8527	0.8428
	ν_{18a}	0.1606	0.1541	0.1438	0.1397	0.1363	0.1335	0.1301
	ν_{8a}	0.9315	0.9255	0.9161	0.9118	0.9070	0.9022	0.8928
S_3	ν_{6a}	0.0974	0.0867	0.0636	0.0521	0.0408	0.0297	0.0083
	ν_{1}	0.9387	0.9502	0.9733	0.9817	0.9892	0.9950	1.0008
	ν_{12}	0.6002	0.5695	0.5096	0.4825	0.4550	0.4288	0.3846
	ν_{19a}	0.4280	0.4202	0.4044	0.3967	0.3875	0.3778	0.3563
	ν_{9a}	0.2644	0.2710	0.2889	0.2975	0.3078	0.3185	0.3413
	ν_{18a}	0.0257	0.0295	0.0342	0.0357	0.0361	0.0355	0.0320
	ν_{8a}	0.9070	0.9064	0.9101	0.9124	0.9154	0.9187	0.9271
S_4	ν_{6a}	0.0238	0.0408	0.0161	0.0043	0.0073	0.0184	0.0392
	ν_{1}	0.0125	0.9286	0.9493	0.9569	0.9635	0.9685	0.9732
	ν_{12}	0.0141	0.5576	0.4982	0.4714	0.4441	0.4183	0.3746
	ν_{19a}	0.0233	0.3918	0.3748	0.3667	0.3571	0.3470	0.3251
	ν_{9a}	0.0468	0.3143	0.3316	0.3398	0.3496	0.3598	0.3815
	ν_{18a}	0.0069	0.0173	0.0218	0.0232	0.0235	0.0230	0.0198
	ν_{8a}	0.0033	0.9069	0.9108	0.9131	0.9161	0.9195	0.9276

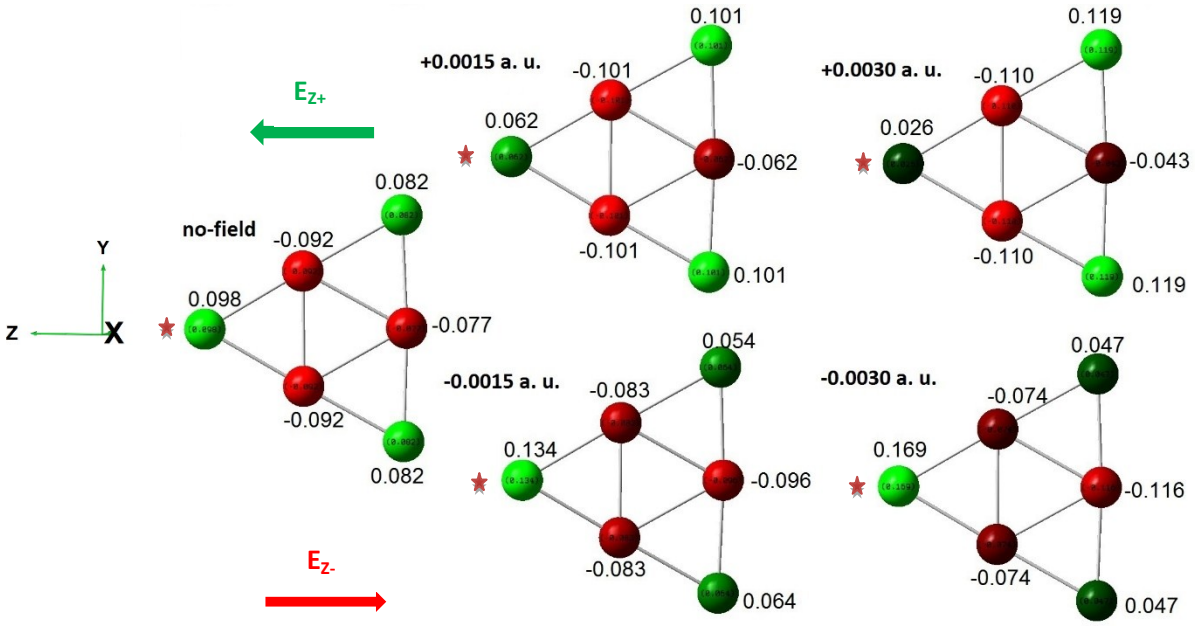

Fig. S1 NPA charge separation of the isolated Ag_6 cluster with respect to the external electric field (the anchoring Ag atom shows with asterisk).

Fig. S2 The highest occupied molecular orbitals of Py-Ag_6 complex, which localize on metal cluster.