Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Probing the electronic and optical properties of silica coated quantum dots with first-principles calculations

Cunku Dong,[a] Xin Li, *[ab] and Jingyao Qi[b]

[a] *Department of Chemistry, Harbin Institute of Technology, Harbin 150090, China. Fax:* +86 451 86403297*; Tel:* +86 451 86282153*; E-mail: Lixin@hit.edu.cn.*

[b] *State Key Lab of Urban Water Resource and Environment, Harbin Institute of Technology, Harbin 150090, China.*

Index **Page**

Table S1. Excitation energies (ΔE in nm) and oscillator strengths (f) of Cd_2Te_2 cluster for B3LYP/ DZVP calculated 10 lowest singlet-singlet excited states at D_{2h} Symmetry.

ΔE	f	transition	weight
898	0.000	HOMO→LUMO	0.690
663	0.000	HOMO→LUMO+1	0.681
644	0.013	HOMO-1→LUMO	0.689
552	0.017	HOMO-2→LUMO	0.655
		HOMO-3→LUMO+1	-0.179
528	0.000	HOMO-3→LUMO	0.663
		HOMO-2→LUMO+1	-0.190
517	0.000	HOMO-1→LUMO+1	0.687
482	0.000	HOMO-3→LUMO	0.190
		HOMO-2→LUMO+1	0.658
362	0.090	HOMO-3→LUMO+1	0.567
		HOMO-2→LUMO+4	0.157
		HOMO→LUMO+2	0.324
314	0.220	HOMO-5→LUMO+1	-0.200
		HOMO-4→LUMO	0.616
		HOMO-1→LUMO+3	0.161
295	0.000	HOMO-5→LUMO	-0.332
		HOMO-4→LUMO+1	0.566
		HOMO-1→LUMO+3	0.219

Table S2. Excitation energies (ΔE in nm) and oscillator strengths (f) of $Cd_2Te_2@(SiO_2)_{24}$ for B3LYP/DZVP&6-31G* calculated 10 lowest singlet-singlet excited states at D_{2h} Symmetry.

ΔE	f	transition	weight
616	0.000	HOMO→LUMO	0.704
558	0.000	HOMO-1→LUMO	0.703
534	0.010	HOMO-2→LUMO	0.701
530	0.000	HOMO→LUMO+1	0.704
485	0.000	HOMO-1→LUMO+1	0.705
468	0.000	HOMO-2→LUMO+1	0.704
459	0.027	HOMO-3→LUMO	0.682
		HOMO→LUMO+2	-0.173
449	0.0021	HOMO-4→LUMO	0.705
410	0.000	HOMO-3→LUMO+1	0.670
		HOMO→LUMO+4	0.216
406	0.0015	HOMO-3→LUMO	0.177
		HOMO→LUMO+2	0.682