Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2015**, *31* (8), 1504–1512
doi: 10.3866/PKU.WHXB201505211

含中氮茚有机太阳能电池染料敏化剂的分子设计

侯丽梅 [1,2]　温　智 [2,3]　李银祥 [2]　胡华友 [2]　阚玉和 [2,3,*]

苏忠民 [1,3,*]

([1] 延边大学理学院化学系, 吉林 延吉　133002; [2] 江苏省低维材料化学重点建设实验室, 淮阴师范学院化学化工学院, 江苏 淮安　223300; [3] 东北师范大学化学学院, 功能材料化学研究所, 长春　130024)

Molecular Design of Indolizine Derivative as Sensitizers for Organic Dye-Sensitized Solar Cells

HOU Li-Mei[1,2]　WEN Zhi[2,3]　LI Yin-Xiang[2]　HU Hua-You[2]

KAN Yu-He[2,3,*]　SU Zhong-Min[1,3,*]

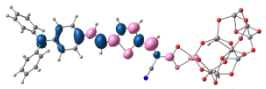
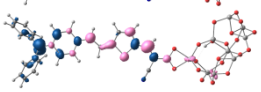
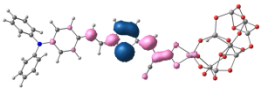
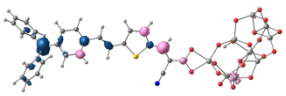
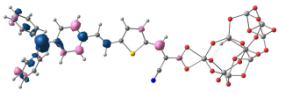
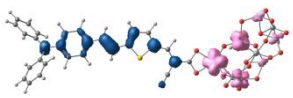
([1]*Department of Chemistry, School of Science and Engineering, Yanbian University, Yanji 133002, Jilin Province, P. R. China*; [2]*Jiangsu Province Key Laboratory for Chemistry of Low-Dimensional Materials, School of Chemistry and Chemical Engineering, Huaiyin Normal University, Huai'an 223300, Jiangsu Province, P. R. China*; [3]*Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, P. R. China*)

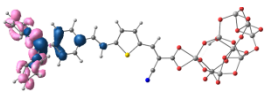
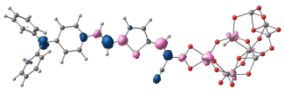
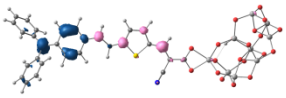
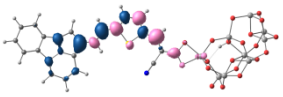
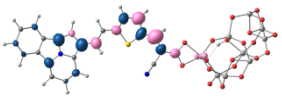
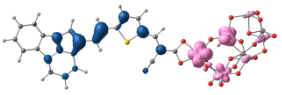
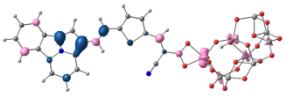
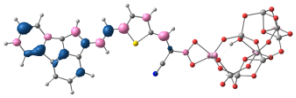
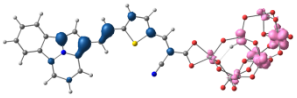
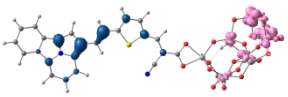
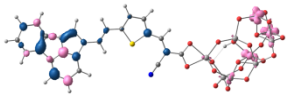
[*]Corresponding authors. SU Zhong-Min, Email: zmsu@nenu.edu.cn; Tel: +86-433-85684009.
KAN Yu-He, Email: kyh@hytc.edu.cn.

Table S1 Computed the length of CT (D_{CT} in Å), transition dipole moment μ_{eg} (a. u.), and spatial overlap index (Λ) of D5, D9 and INI1- INI 9 in ethanol solvent

	B3LYP			ωB97XD		
	D_{CT}	Λ	μ_{eg}	D_{CT}	Λ	μ_{eg}
D5	6.2	0.782	21.6	4.2	0.889	23.6
D9	6.5	0.762	22.0	4.4	0.878	24.8
INI-1	5.2	0.750	19.3	3.0	0.919	17.1
INI-2	4.6	0.837	25.5	3.9	0.878	24.7
INI-3	5.7	0.784	18.0	3.5	0.914	17.9
INI-4	5.8	0.770	17.8	4.2	0.876	20.7
INI-5	5.3	0.758	17.1	3.0	0.921	10.5
INI-6	5.7	0.727	10.8	3.4	0.897	14.0
INI-7	6.2	0.777	18.2	4.0	0.891	22.6
INI-8	6.8	0.743	21.1	3.2	0.922	21.9
INI-9	5.5	0.748	9.4	3.9	0.861	17.4

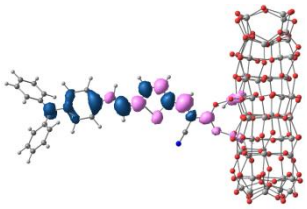
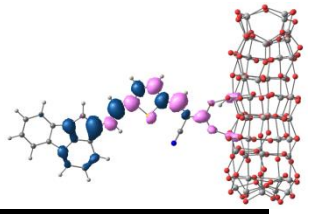
Table S2 Calculated the lowest excitation energy (*E*, in eV), absorption wavelength (λ in nm), oscillator strength (*f*) and transition nature of D5-$(TiO_2)_9$ and INI2-$(TiO_2)_9$ at PCM-*ω*B97XD /6-31g* level of theory in ethanol solvent

State	*E*	λ	*f*	Transition contributions	CDD[a]
				D5-$(TiO_2)_9$	
$S_0 \rightarrow S_1$	2.57	482	2.2562	H-1→L (21%), H→L (70%)	
$S_0 \rightarrow S_2$	3.75	330	0.0771	H-4→L (10%), H-1→L (50%), H→L+18 (14%)	
$S_0 \rightarrow S_3$	4.35	285	0.0560	H-7→L (86%)	
$S_0 \rightarrow S_4$	4.38	283	0.0771	H→L (10%), H→L+18 (25%), H→L+29 (15%)	
$S_0 \rightarrow S_6$	4.46	278	0.0528	H→L+29 (41%)	
$S_0 \rightarrow S_7$	4.60	270	0.0453	H→L+1 (21%), H→L+3 (14%), H→L+5 (15%)	

$S_0 \rightarrow S_9$	4.67	265	0.2647	H-1→L+31 (10%), H→L+29 (13%), H→L+31 (59%)	
$S_0 \rightarrow S_{12}$	4.83	257	0.0695	H-8→L (10%), H-4→L (26%), H-1→L+18 (11%)	
$S_0 \rightarrow S_{40}$	5.23	237	0.0815	H-6→L (16%), H-3→L (17%), H→L+41 (26%)	
		INI2-$(TiO_2)_9$			
$S_0 \rightarrow S_1$	2.32	534	1.9193	H→L (85%)	
$S_0 \rightarrow S_3$	3.92	316	0.183	H-3→L (11%), H-2→L (19%), H-1→L (39%)	
$S_0 \rightarrow S_6$	4.37	284	0.0122	H→L+1 (24%), H→L+3 (16%), H→L+5 (22%)	
$S_0 \rightarrow S_8$	4.54	273	0.0967	H→L+23 (22%), H→L+28 (10%)	
$S_0 \rightarrow S_{21}$	4.93	252	0.2776	H-3→L (33%), H-2→L+13 (10%), H→L+28 (12%)	
$S_0 \rightarrow S_{24}$	4.97	250	0.2353	H→L+2 (14%), H→L+4 (15%)	
$S_0 \rightarrow S_{94}$	5.68	218	0.1322	H→L+12 (24%), H→L+14 (16%)	
$S_0 \rightarrow S_{95}$	5.69	218	0.4586	H-2→L+28 (12%), H-1→L+28 (13%)	

[a] charge difference density(contour value 0.001258 a.u.)

Table S3 Calculated the lowest excitation energy (*E*, in eV), absorption wavelength (λ in nm), oscillator strength (*f*) and transition nature of D5-$(TiO_2)_{48}$ and INI2-$(TiO_2)_{48}$ at PCM-ωB97XD /6-31g* level of theory in ethanol solvent

State	*E*	λ	*f*	Transition contributions	CDD[a]
			D5-$(TiO_2)_{48}$		
$S_0 \rightarrow S_1$	2.44	508	2.4316	H-1→L (19%), H→L (68%)	
			INI2-$(TiO_2)_{48}$		
$S_0 \rightarrow S_1$	2.23	554	2.0658	H→L (80%)	

[a] charge difference density(contour value 0.001258 a.u.)

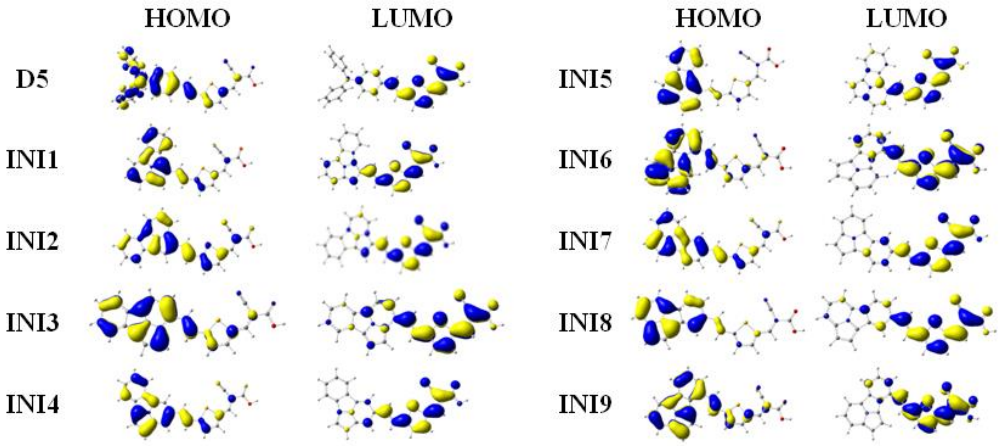


Fig.S1 Frontier molecular orbitals (isovalue 0.03 a.u.) of D5 and INI1-9 at ωB97XD /6-31g* level

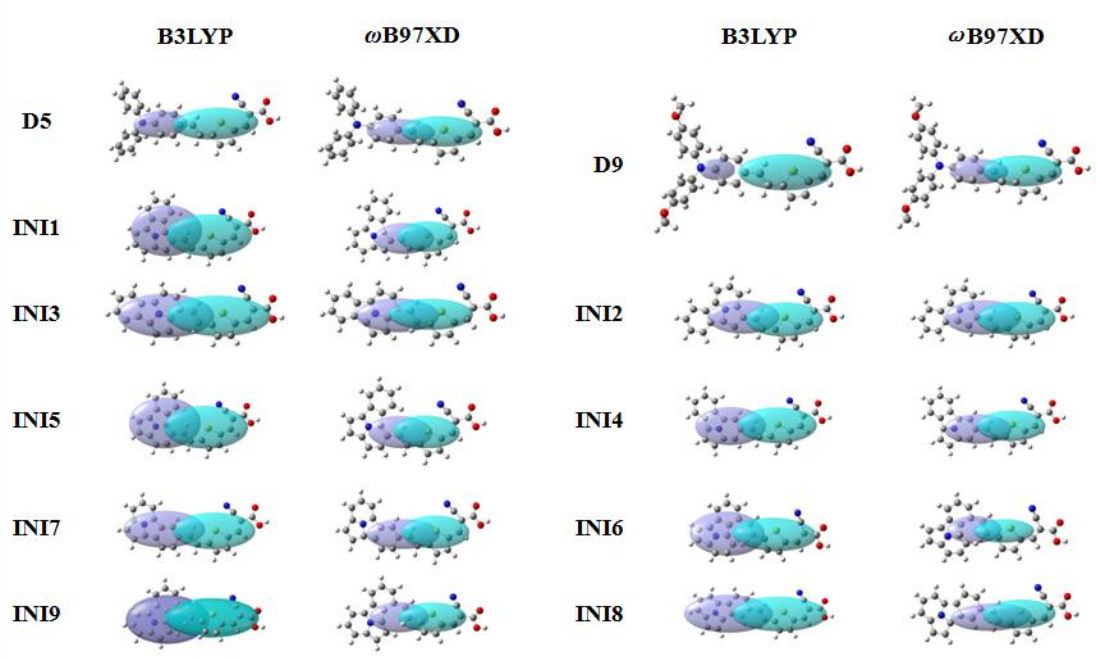


Fig. S2 Computed centroids of charge C_- (blue) and C_+ (green) of D5, D9 and INI1- INI9 (isocontour value 0.00055 a.u.)

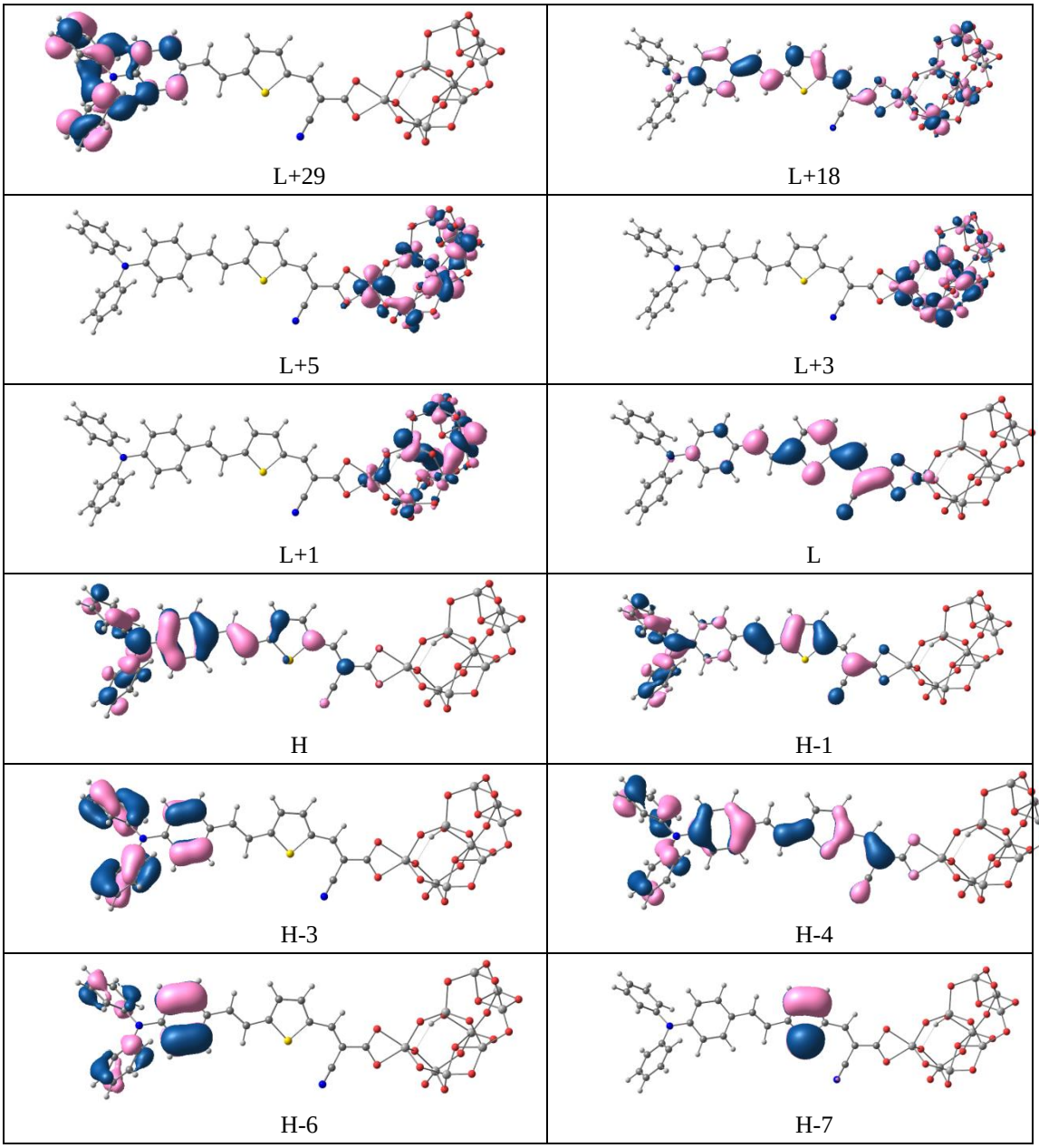


Fig.S3 Relative MOs of the excited state for D5-$(TiO_2)_9$

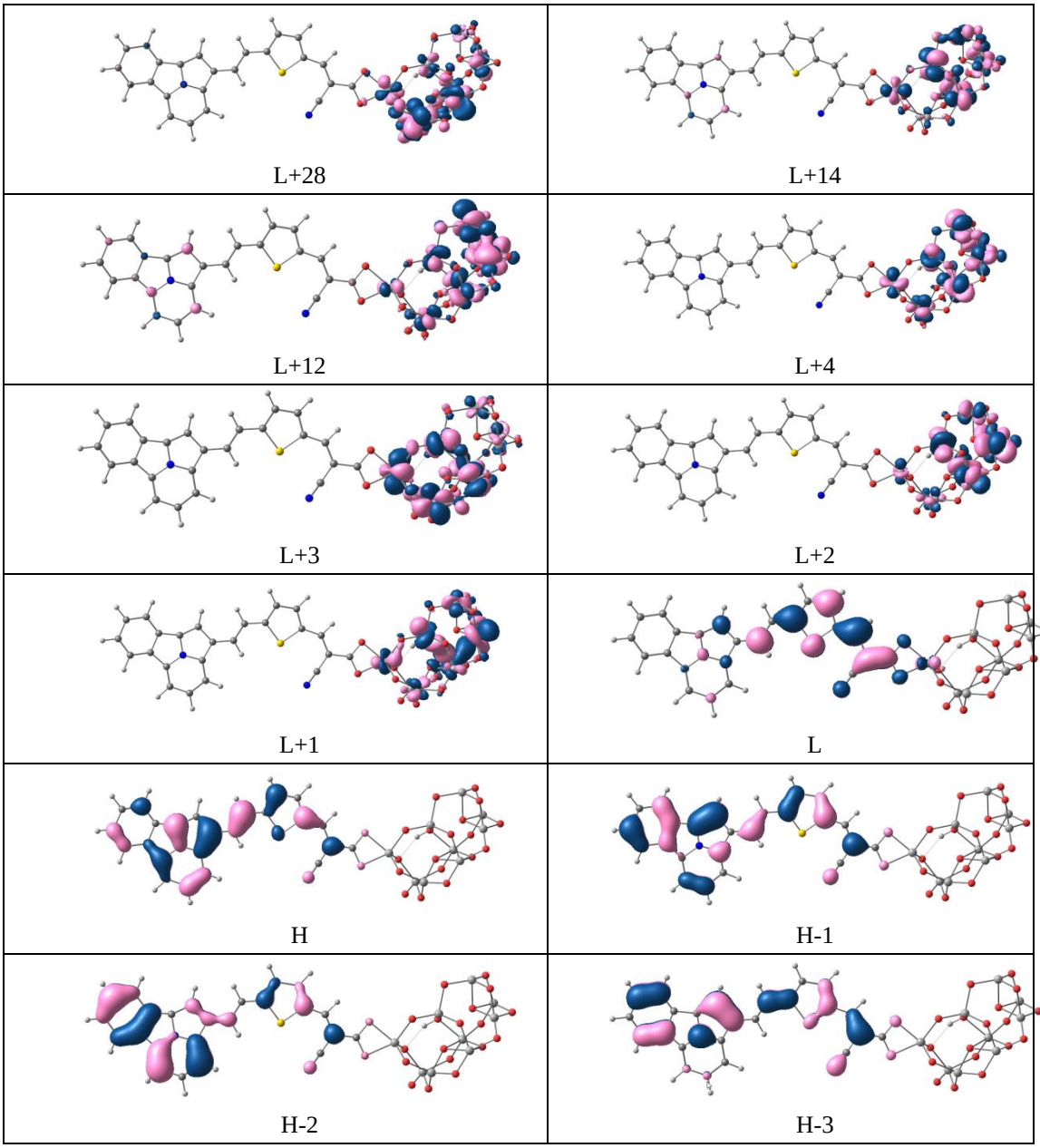


Fig.S4 Relative MOs of the excited state for INI2-$(TiO_2)_9$