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

Optical absorption of warped nanographenes tuned by five- and seven-membered carbon rings

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Tabel S2 Compositions of HOMO to LUMO transitions.

Fig. S1 Optimized structure of $C_{80}H_{30}$. Values in red are the dihedral angles (in degree) of the structure obtained with B3LYP/def-TZVP.

Fig. S2 Projected density of states (PDOS) of $C_{80}H_{30}$ and $C_{78}H_{80}$.

Fig. S3 The UV/Vis absorption spectra of $C_{80}H_{30}$ caculated with various functionals of B3LYP, Cam-B3LYP, PBE, PBE0, M06-2X and TPSSh.

Fig. S4 HOMO and LUMO orbitals of **a**–**e**.

Fig. S5 HOMO and LUMO orbitals of **a´**–**e´**.

Fig. S6 HOMO and LUMO contours of the model molecules shown in Fig. 4.

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	HOMO	LUMO	Gaps		HOMO	LUMO	Gaps
$C_{80}H_{30}$	-5.336	-2.329	3.007				
$C_{78}H_{30}$	-5.168	-2.263	2.905				
a	-5.276	-2.406	2.870	**a'**	-5.355	-2.396	2.959
b1	-5.256	-2.429	2.827	**b1'**	-5.221	-2.332	2.889
b2	-5.214	-2.402	2.812	**b2'**	-5.363	-2.393	2.970
c	-5.327	-2.496	2.830	**c'**	-5.416	-2.410	3.005
d	-5.250	-2.454	2.795	**d'**	-5.338	-2.365	2.973
e	-5.398	-2.513	2.884	**e'**	-5.500	-2.408	3.093

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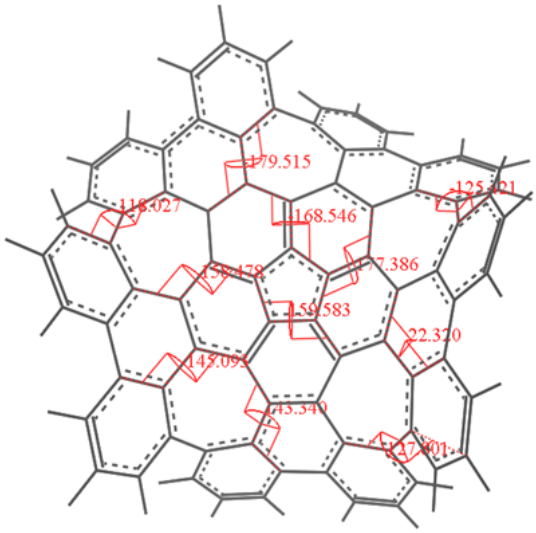
	α			β			γ	
$C_{80}H_{30}$	485.56nm		f=0.1772	435.53nm		f=0.5851	335.72nm	f=0.2725
HOMO:255	254 → 257		0.192	252 → 256		-0.206	249 → 257	-0.114
LUMO:256	255 → 256		0.668	253 → 256		-0.195	252 → 258	-0.148
	254 → 256		0.366	253 → 259		-0.396		
	255 → 257		0.507	255 → 260		-0.101		
	255 → 261		-0.105					
	255 → 263		0.431					
	255 → 265		-0.105					
$C_{78}H_{30}$	443.16nm		f=1.8478	443.16nm		f=1.8478	298.22nm	f=0.1942
HOMO:249	248 → 250		0.339	248 → 250		0.339	244 → 254	0.119
LUMO:250	248 → 251		0.363	248 → 251		0.363	247 → 253	0.354
	249 → 250		0.360	249 → 250		0.360	248 → 261	0.160
	249 → 251		-0.339	249 → 251		-0.339	248 → 262	0.338
	248 → 263		-0.155					
	249 → 261		0.349					
	249 → 262		-0.163					
a	514.02nm		f=0.1315	458.77nm		f=0.6236	389.45nm	f=0.1076
HOMO:248	246 → 249		-0.108	246 → 249		0.171	241 → 249	-0.174
LUMO:249	247 → 250		0.242	247 → 249		0.433	242 → 249	-0.352
	248 → 249		0.636	248 → 250		0.509	243 → 249	-0.229
	244 → 250		0.424					
	247 → 251		0.121					
	247 → 253		-0.111					
	248 → 252		0.130					
b1	522.13nm		f=0.0657	464.41nm		f=0.5894	351.26nm	f=0.1434
HOMO:241	240 → 242		0.225	238 → 242		-0.268	234 → 242	-0.100
LUMO:242	240 → 243		0.255	238 → 243		0.125	238 → 244	-0.112
	241 → 242		0.569	239 → 242		-0.111	238 → 245	-0.125
	241 → 243		-0.209	240 → 242		0.378	239 → 244	-0.276
	241 → 243		0.475	239 → 247		0.100		
	240 → 246		-0.139					
	240 → 248		0.260					
	241 → 246		-0.228					
	241 → 248		0.380					
	241 → 249		-0.124					
b2	518.76nm		f=0.2384	456.17nm		f=0.5224	389.37nm	f=0.0970
HOMO:241	240 → 243		-0.182	240 → 242		-0.471	236 → 242	0.514
LUMO:242	241 → 242		0.669	241 → 243		0.491	237 → 243	0.103
	241 → 244		0.137					
	241 → 245		0.392					

	241 → 249	-0.105							
c	524.38nm	f=0.1027	454.04nm	f=0.7295	395.05nm	f=0.1126			
HOMO:234	232 → 235	-0.161	231 → 236	0.186	230 → 235	0.599			
LUMO:235	233 → 236	-0.303	232 → 235	0.104	232 → 236	-0.213			
	234 → 235	0.611	233 → 236	0.579	233 → 238	0.250			
	234 → 235	0.319							
d	531.04nm	f=0.0307	458.19nm	f=0.5001	389.91nm	f=0.1008			
HOMO:227	226 → 228	-0.225	224 → 228	0.370	223 → 228	0.236			
LUMO:228	226 → 229	-0.317	224 → 229	-0.369	223 → 229	0.461			
	227 → 228	0.501	226 → 228	-0.301	225 → 230	-0.109			
	227 → 229	-0.288	226 → 229	0.161	226 → 230	0.198			
	227 → 228	0.136	227 → 232	-0.348					
	227 → 229	0.245							
e	454.53nm	f=1.0727	454.53nm	f=1.0727	339.36nm	f=0.5165			
HOMO:220	219 → 221	0.316	219 → 221	0.316	214 → 221	-0.116			
LUMO:221	219 → 222	0.375	219 → 222	0.375	215 → 222	-0.111			
	220 → 221	-0.373	220 → 221	-0.373	217 → 223	0.319			
	220 → 222	0.317	220 → 222	0.317	218 → 224	0.488			
	219 → 225	0.208							
	220 → 226	0.220							
a'	492.35nm	f=0.1948	432.78nm	f=0.4404	344.76nm	f=0.1990			
HOMO:256	255 → 258	-0.112	253 → 257	0.135	248 → 258	0.104			
LUMO:257	256 → 257	0.680	254 → 257	-0.151	253 → 259	0.250			
	255 → 257	-0.235	253 → 260	0.478					
	255 → 258	0.135	254 → 259	0.240					
	256 → 258	0.601	254 → 261	0.143					
	256 → 262	-0.210							
	256 → 263	0.111							
b1'	504.94nm	f=0.1879	454.06nm	f=0.2423	422.49nm	f=0.2540			
HOMO:257	256 → 259	0.121	254 → 258	-0.156	254 → 258	-0.378			
LUMO:258	257 → 258	0.683	255 → 258	-0.193	255 → 259	0.341			
	256 → 258	0.493	256 → 259	0.428					
	257 → 259	0.326	257 → 259	-0.126					
	257 → 260	-0.256							
b2'	489.51nm	f=0.2493	436.17nm	f=0.3371	414.71nm	f=0.3319			
HOMO:257	257 → 258	0.688	255 → 258	-0.229	255 → 258	0.140			
LUMO:258	256 → 258	-0.225	256 → 259	0.647					
	256 → 259	0.142	257 → 259	-0.114					
	257 → 259	0.593							
c'	495.29nm	f=0.0346	412.12nm	f=0.3581	383.56nm	f=0.2260			
HOMO:258	256 → 259	0.162	255 → 259	0.222	252 → 259	0.317			
LUMO:259	257 → 259	0.359	257 → 260	0.594	254 → 259	0.153			
	258 → 259	0.573	258 → 260	-0.180	255 → 260	0.121			
	258 → 261	0.126	256 → 260	0.183					

	257	→	261	0.210					
	258	→	261	0.482					
d'	499.15nm			f=0.0650	432.12nm			f=0.3956	373.16nm			f=0.1807
HOMO:259	258	→	261	0.207	256	→	260	0.278	253	→	260	0.409
LUMO:260	259	→	260	0.648	257	→	260	0.194	254	→	260	-0.234
	259	→	261	0.156	257	→	261	0.359	255	→	260	0.131
	258	→	260	0.133	255	→	261	0.117				
	258	→	261	-0.337	257	→	262	0.417				
	259	→	261	0.166								
	259	→	262	-0.263								
e'	445.2nm			f=0.1954	426.39nm			f=0.5049	366.25nm			f=0.2194
HOMO:260	257	→	261	-0.281	257	→	261	0.416	251	→	261	0.524
LUMO:261	257	→	262	-0.116	258	→	262	0.388	253	→	261	0.146
	258	→	261	-0.249	258	→	263	-0.110	255	→	262	-0.138
	258	→	262	0.408	259	→	262	-0.323	257	→	263	0.177
	259	→	261	0.154	260	→	262	0.175	258	→	263	0.224
	260	→	262	-0.359	258	→	264	0.109				
	259	→	263	-0.106								
	260	→	263	-0.138								



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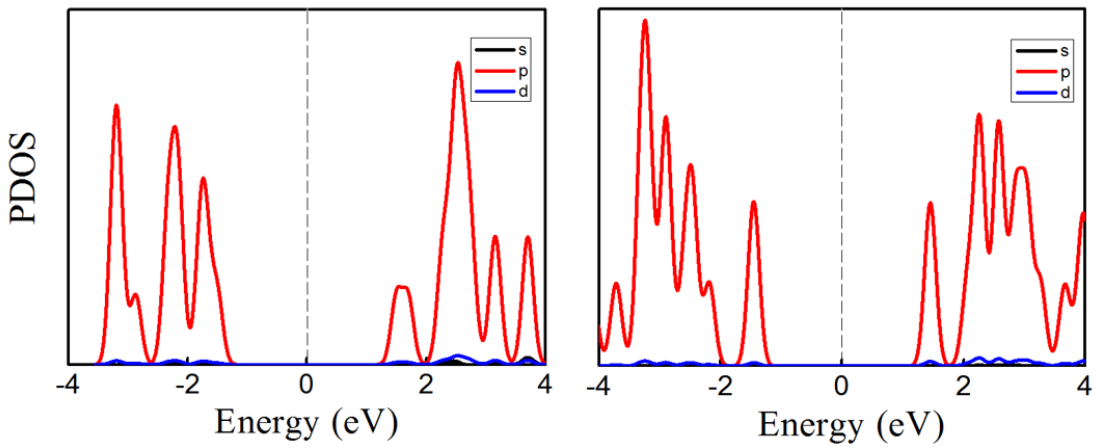

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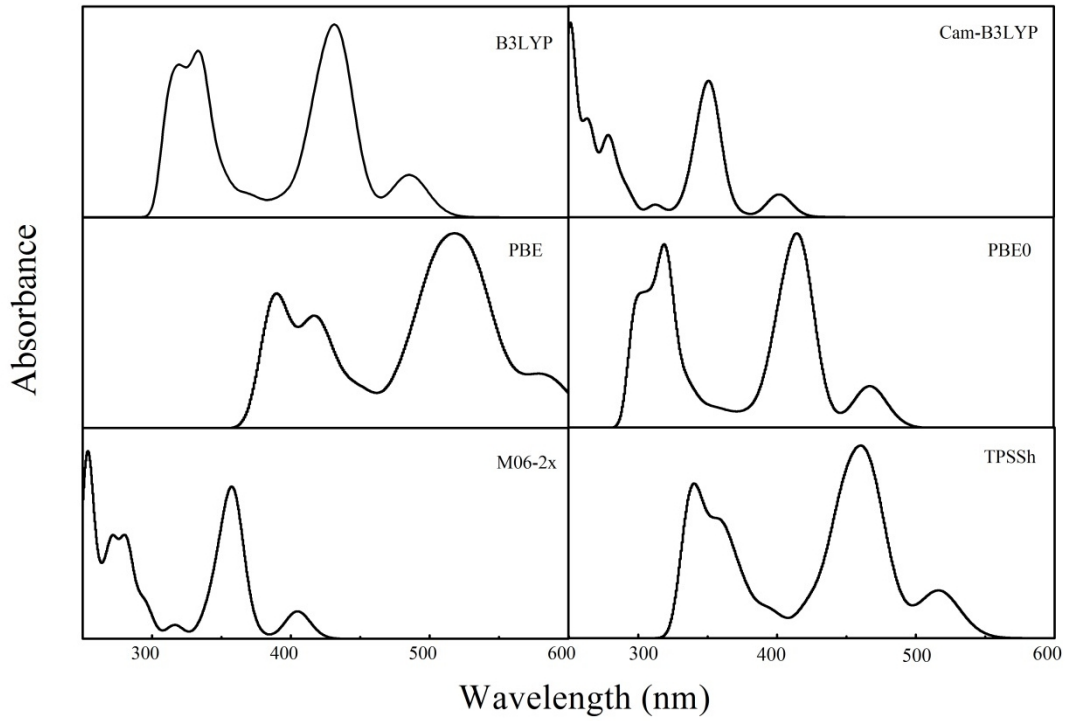

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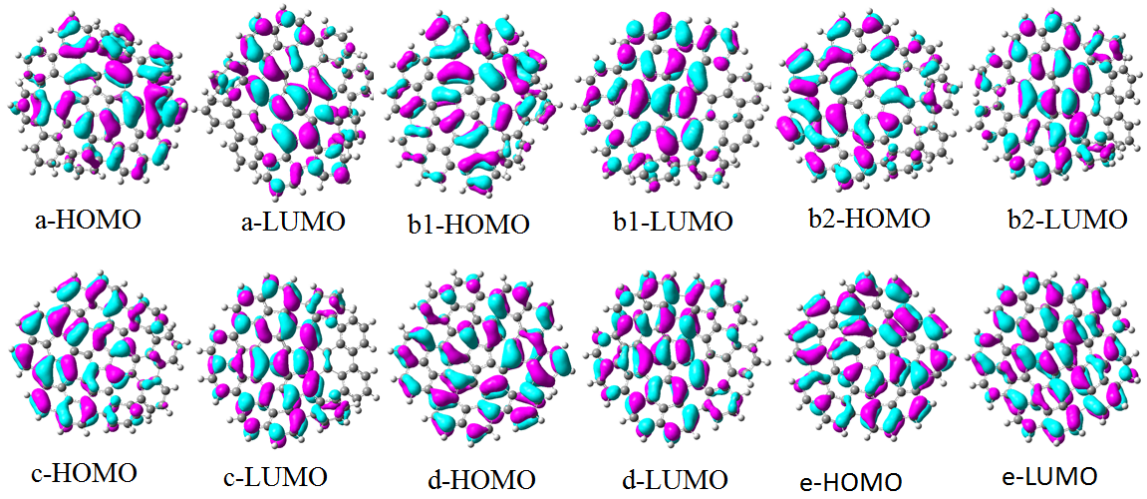

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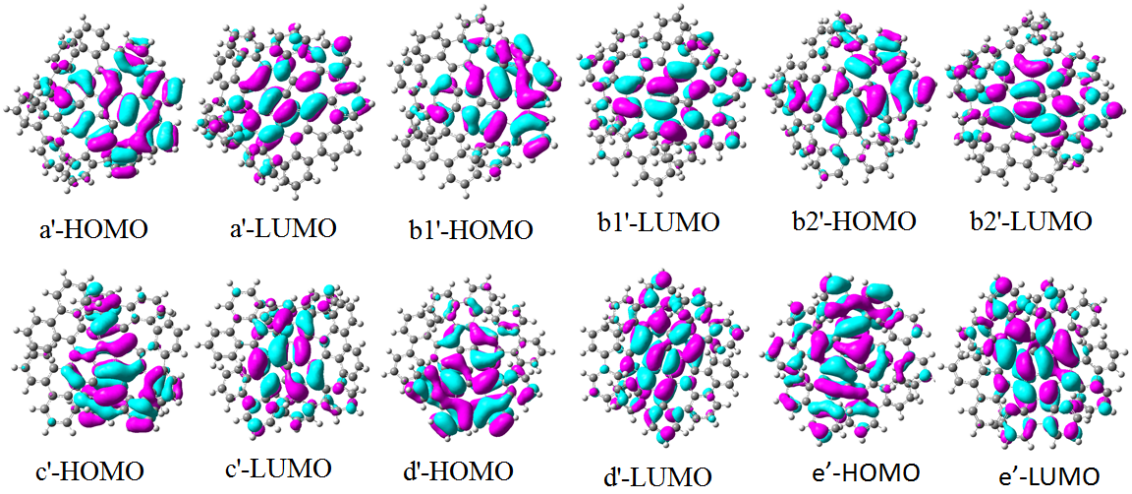
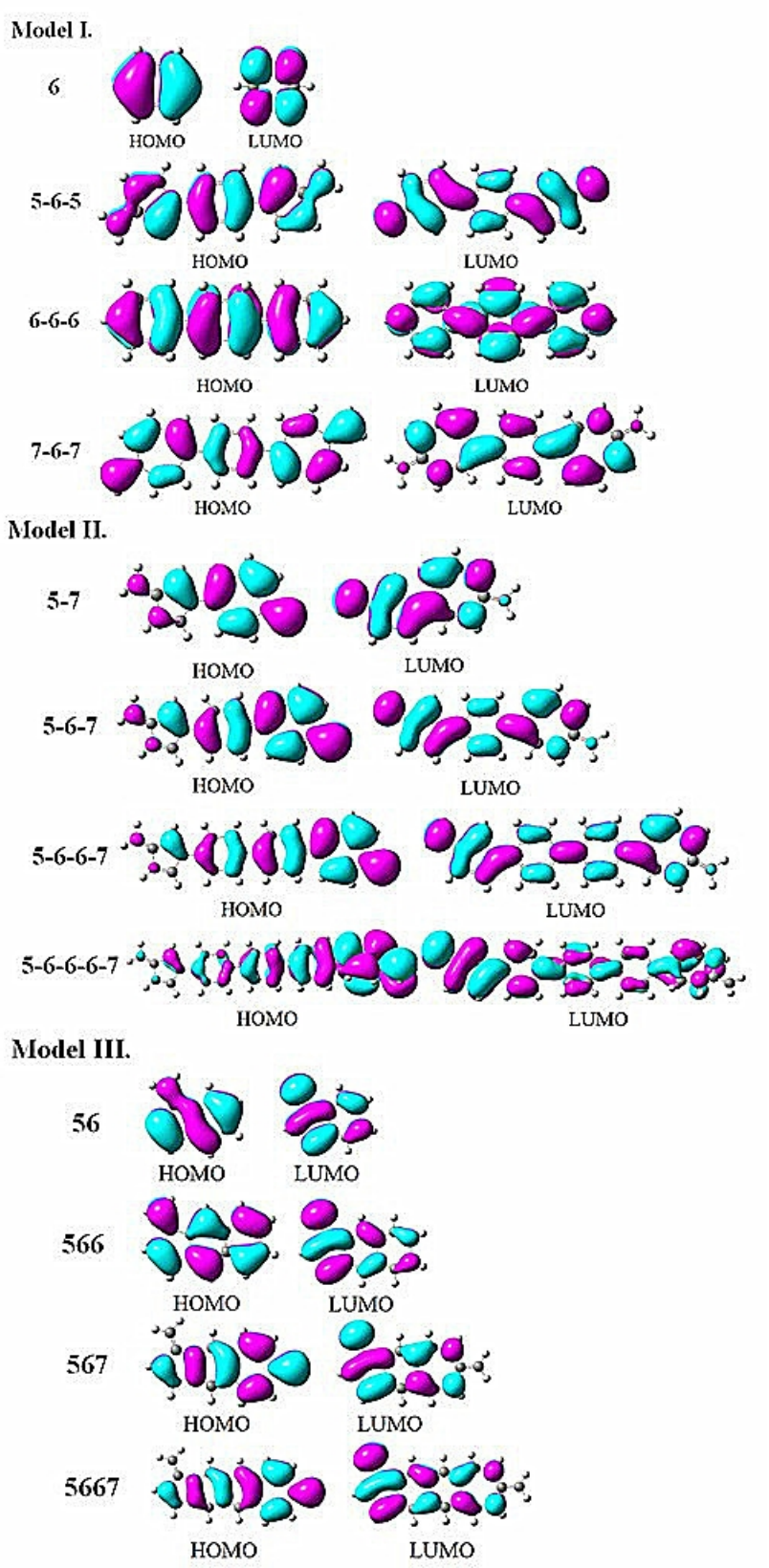


Fig. S5 HOMO and LUMO orbitals of **a´**–**e´**.



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