Supporting Information for:

Strong Tunable Visible Absorption Predicted for Polysilo-acenes using TDDFT Calculations

K. L. Dimuthu M. Weerawardene and Christine M. Aikens*

Department of Chemistry, Kansas State University, Manhattan, KS 66506, USA

*cmaikens@ksu.edu, 1-785-532-0954, fax: 1-785-532-6666

Table S1. TDDFT energy and wavelength of the β-band of polysilo-acenes with various exchange-correlation functionals

Number of fused rings	BP86/TZP		PBE/TZP		LB94/TZP		SAOP/TZP	
	Energy (eV)	Wavelength (nm)	Energy (eV)	Wavelength (nm)	Energy (eV)	Wavelength (nm)	Energy (eV)	Wavelength (nm)
2	2.561	484.7	2.563	484.4	2.445	507.7	2.570	483.1
3	2.184	568.4	2.186	567.9	2.086	595.0	2.197	565.0
4	1.919	646.9	1.878	661.1	1.855	669.1	1.936	641.4
5	1.714	724.5	1.716	723.7	1.649	753.1	1.728	718.4
6	1.570	790.8	1.522	816.0	1.476	841.2	1.571	790.1

Table S2. The excitation energies, oscillator strengths, transitions involved, weights and the transition dipole moments corresponding to α and β peaks of planar polysilo-acenes.

Number of fused rings in the polysilo-acene	Peak energy (eV)		Oscillator Strength (a.u.)	Transitions	Weight	Transition dipole moment (a.u.)
2	α peak	1.88	0.0000134	HOMO→LUMO+1	0.4941	-3.3585
				HOMO-1→LUMO	0.5037	3.3700
	β peak	2.69	0.699	HOMO→LUMO+1	0.4721	-2.7576
				HOMO-1→LUMO	0.4597	-2.7077
3	α peak	1.60	0.0000198	HOMO→LUMO+1	0.4778	-4.2782
				HOMO-1→LUMO	0.5204	4.3850
	β peak	2.30	1.101	HOMO→LUMO+1	0.4846	3.5856
				HOMO-1→LUMO	0.4403	3.3565
4	α peak	1.41	0.000263	HOMO→LUMO+2	0.4621	5.0119
				HOMO-2→LUMO	0.5362	-5.2358
	β peak	2.03	1.435	HOMO→LUMO+2	0.4857	4.2898
				HOMO-2→LUMO	0.4118	3.8306
5	α peak	1.29	0.000950	HOMO→LUMO+2	0.4476	-5.9658
				HOMO-2→LUMO	0.5507	5.6104
	β peak	1.82	1.612	HOMO→LUMO+2	0.4732	4.8652
				HOMO-2→LUMO	0.3750	4.1523
6	α peak	1.21	0.00201	HOMO→LUMO+2	0.4343	6.0972
				HOMO-3→LUMO	0.5638	-6.5895
	β peak	1.65	1.653	HOMO→LUMO+2	0.4559	5.3454
				HOMO-3→LUMO	0.3383	4.3685

Table S3. Analysis of the p-band of planar $Si_{10}H_8$ at the BP86/TZP level of theory.

Peak energy (eV)	Oscillator Strength (a.u.)	Transitions	Weight	Transition dipole moment (a.u.)
1.80	0.0235	HOMO→LUMO	0.9090	-2.8263
		HOMO-2→LUMO+2	0.0410	0.8220
		HOMO-1→LUMO+1	0.0392	0.7003
2.70	0.0689	HOMO-1→LUMO+1	0.8569	2.6741
		HOMO-2→LUMO+2	0.0937	-1.0149
		HOMO→LUMO	0.0163	0.3093
3.52	0.3005	HOMO-2→LUMO+2	0.8220	-2.6335
		HOMO-1→LUMO+1	0.0654	-0.6469
		HOMO→LUMO	0.0525	-0.4859

Table S4. The excitation energy of the strongest p-band peak of planar and buckled polysilo-acenes.

Number of fused rings in the polysilo-acene	Peak energy (eV)	
	Planar Polysilo-acenes	Buckled Polysilo-acenes
2	3.518	3.323
3	3.637	3.374
4	3.686	3.392
5	3.728	3.417
6	3.733	3.421

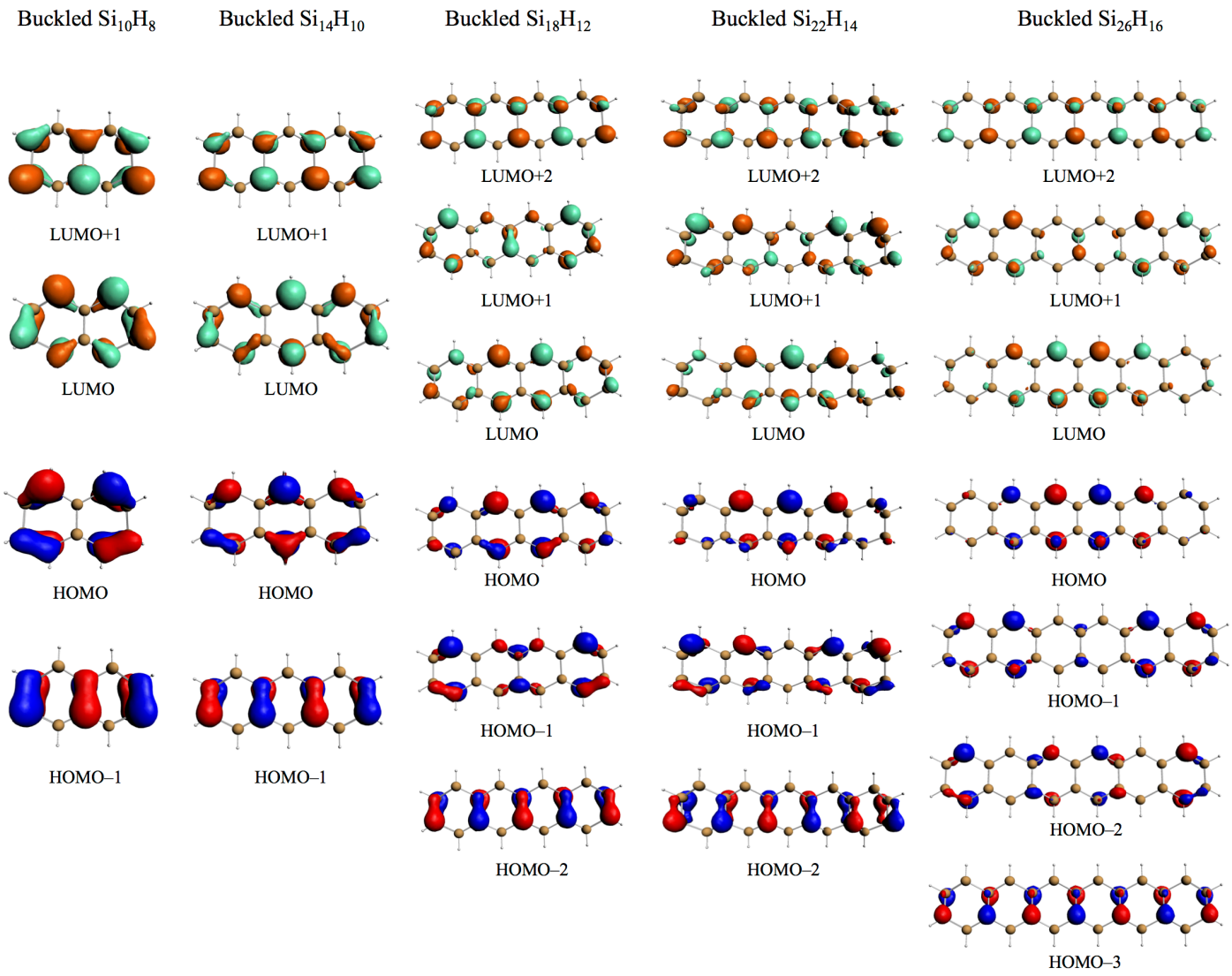

Figure S1. Orbitals involved in transitions contributing to α and β peaks of buckled polysilo-acenes. In longer systems, HOMO-2 or HOMO-3 and LUMO+2 orbitals have the same character as HOMO-1 and LUMO+1 of the shorter polysilo-acenes.