Supporting Information

Geometry, electronic structure, and optical properties of boron cages: A first-principles DFT study

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Oscillator strengths and the configurations with significantly large coefficients in the TDDFT wave functions of the excited states giving rise to various peaks in the dynamically stable clusters.

1. B_{32}

Peak	Energy (eV)	OS	Configuration
I	2.5953	0.0163	H-1:L+3
	2.5963	0.0164	H-2:L+3
	2.5966	0.0164	H-2:L+4

2. B_{42}

Peak	Energy (eV)	OS	Configuration
I	1.3164	0.0022	H:L
	1.4240	0.0039	H-1:L
II	2.0928	0.0063	H-1:L+2
	2.1549	0.0018	H-2:L+2
III	2.4337	0.0034	H-5:L
	2.4856	0.0055	H-1:L+5
IV	2.6277	0.0037	H-1:L+6
	2.6527	0.0033	H-5:L+1
	2.7032	0.0035	H-2:L+2
	2.7609	0.0055	H:L+7
	2.8176	0.0034	H-1:L+7
	2.9111	0.0081	H-3:L+3
	2.9703	0.0061	H-8:L

	2.9929	0.0032	H:L+8
	3.0012	0.0047	H-4:L+2
V	3.1123	0.0037	H-5:L+1
	3.1563	0.0062	H-3:L+5
	3.1654	0.0045	H-1:L+9
	3.2083	0.0044	H-4:L+3
	3.2330	0.0039	H:L+10
	3.3083	0.0058	H-10:L
	3.3285	0.0055	H-1:L+10
	3.3742	0.0044	H-4:L+4
	3.4326	0.0049	H-1:L+11
	3.4588	0.0097	H-5:L+4
	3.4765	0.0123	H-3:L+7
	3.5145	0.0048	H-2:L+11
VI	3.8207	0.0047	H:L+14
	3.8310	0.0120	H:L+13
	3.8467	0.0081	H-3:L+9
	3.8803	0.0046	H-8:L+3
	3.8900	0.0067	H-7:L+4
	3.8958	0.0064	H-1:L+13
	3.9187	0.0027	H-1:L+14
	3.9312	0.0075	H-1:L+14
	3.9448	0.0027	H-9:L+2
VII	3.9630	0.0057	H-4:L+8
	3.9695	0.0022	H-2:L+13
	3.9799	0.0062	H-2:L+13
	3.9847	0.0063	H-4:L+8
	4.0037	0.0064	H-6:L+7
	4.0097	0.0107	H-2:L+14

3. B_{60}

Peak	Energy (eV)	OS	Configuration
I	1.2632	0.0037	H-2:L
	1.4624	0.0029	H-4:L
	1.5633	0.0164	H-2:L+2
II	1.8151	0.0109	H-2:L+3
	1.8451	0.0092	H-4:L+2
	2.0052	0.0053	H-4:L+3
III	2.1232	0.0055	H:L+5
	2.1750	0.0048	H-7:L
	2.2082	0.0039	H-1:L+3

	2.2353	0.0059	H-2:L+4
	2.3377	0.0081	H:L+6
	2.4155	0.0089	H-3:L+3
	2.4420	0.0085	H-7:L+1
	2.5099	0.0117	H-3:L+5
	2.5315	0.0096	H-1:L+6
	2.5927	0.0127	H:L+8
	2.6842	0.0051	H-3:L+6
	2.7297	0.0044	H-10:L
	2.7669	0.0071	H-10:L

4. B_{72}

Peak	Energy (eV)	OS	Configuration
I	0.52467	0.0028	H-2:L
	0.52945	0.0030	H-2:L+1
	0.78933	0.0069	H-5:L
	0.81205	0.0058	H-4:L+2
	0.81246	0.0056	H-5:L+2
II	1.27488	0.0039	H-3:L+5
	1.27568	0.0037	H-3:L+6
	1.32940	0.0265	H-2:L+4
	1.43608	0.0034	H-4:L+3
	1.43626	0.0030	H-5:L+3
	1.53923	0.0187	H-4:L+4
	1.54107	0.0179	H-5:L+5
	1.58052	0.0087	H-5:L+5
	1.76986	0.0043	H-1:L+7
	1.77269	0.0043	H-1:L+10

5. B_{92} (Icosahedron)

Peak	Energy (eV)	OS	Configuration
I	1.60202	0.0352	H-2:L
	1.6020	0.0352	H-1:L+1
	1.6020	0.0354	H:L+3

6. B_{122}

Peak	Energy (eV)	OS	Configuration
I	0.8744767282	0.0032	H:L+3
	0.9134619097	0.0024	H:L+4
	0.9150799690	0.0024	H-5:L
	0.9750327149	0.0022	H-6:L
	1.0258835720	0.0043	H:L+5
	1.0973411310	0.004	H-3:L+1
	1.1112482070	0.0041	H-4:L+1
	1.1618797210	0.0025	H:L+6
	1.2385290090	0.0030	H-2:L+4
	1.2446211950	0.0046	H-6:L+1
	1.3523285380	0.0023	H-6:L+2
	1.3575852160	0.0047	H-6:L+3
	1.3969734200	0.0038	H-3:L+5
	1.4214783540	0.0020	H-5:L+4
	1.4291136640	0.0030	H-9:L
	1.4352679320	0.0031	H-6:L+4
	1.4666956690	0.0039	H-10:L
	1.5050825470	0.0036	H-7:L+1
	1.5104917640	0.0030	H-5:L+5
	1.5332812070	0.0021	H-6:L+5
	1.5651604490	0.0043	H-4:L+6
	1.5822381960	0.0034	H-11:L
	1.6036239410	0.0020	H:L+9
	1.6285851180	0.0034	H-7:L+3