Supplementary material for
Large-scale first principles configuration interaction calculations of optical absorption in aluminum clusters

Ravindra Shinde[*] and Alok Shukla[†]
Department of Physics, Indian Institute of Technology Bombay, Mumbai, Maharashtra 400076, INDIA.

In this document, we present the plots of the most important molecular orbitals of the isomers of aluminum clusters considered in this work, and depicted in Fig. 1 of the paper. Furthermore, we also present their ground and excited state CI wave functions, energies, and oscillator strengths corresponding to various peaks in their photoabsorption spectra discussed in section III of the paper.

I. MOLECULAR ORBITALS OF ALUMINUM CLUSTERS

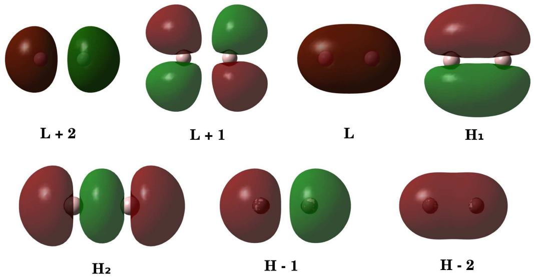

Figure 1: Molecular orbitals of aluminum dimer. H and L stands for HOMO and LUMO respectively, and H_1 and H_2 are singly occupied degenerate molecular orbitals.

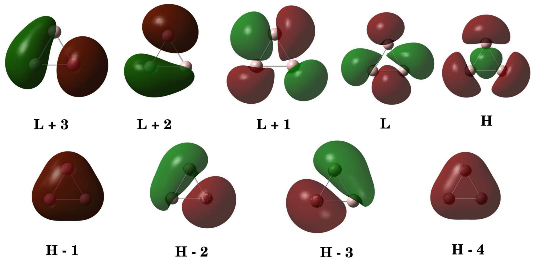

Figure 2: Molecular orbitals of equilateral triangular aluminum trimer. H and L stands for HOMO and LUMO respectively. $(H-2, H-3)$, $(L, L+1)$ and $(L+2, L+3)$ are degenerate pairs.

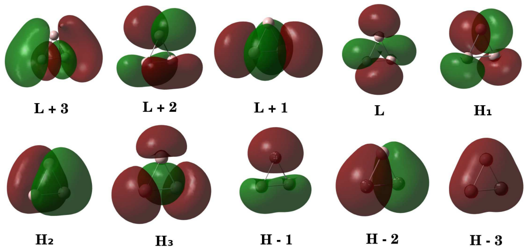

Figure 3: Molecular orbitals of isosceles triangular aluminum trimer. H and L stands for HOMO and LUMO respectively, and H_1, H_2, and H_3 are singly occupied molecular orbitals.

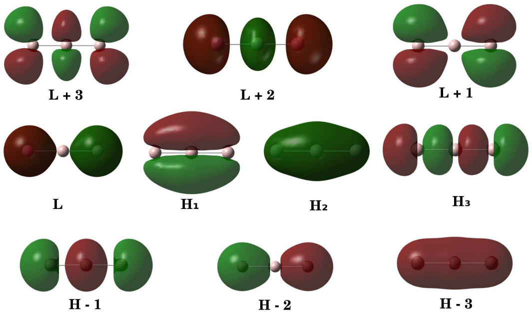

Figure 4: Molecular orbitals of linear aluminum trimer. H and L stands for HOMO and LUMO respectively, and H_1, H_2, and H_3 are singly occupied molecular orbitals.

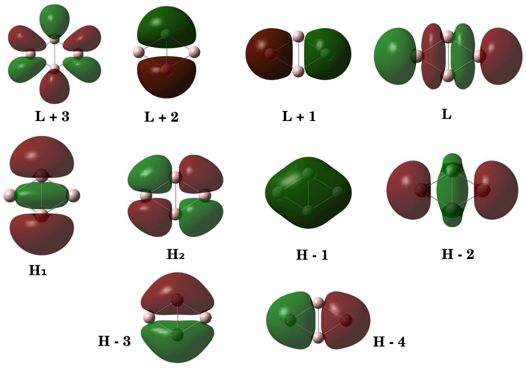

Figure 5: Molecular orbitals of rhombus-shaped aluminum tetramer. H and L stands for HOMO and LUMO respectively, and H_1 and H_2 are singly occupied molecular orbitals.

---

[*] ravindra.shinde@iitb.ac.in
[†] shukla@phy.iitb.ac.in

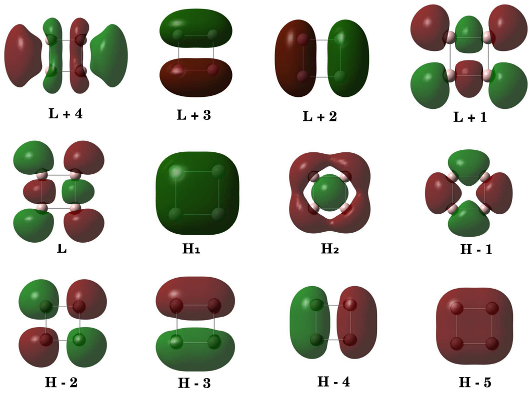

Figure 6: Molecular orbitals of square-shaped aluminum tetramer. H and L stands for HOMO and LUMO respectively, and H_1 and H_2 are singly occupied molecular orbitals.

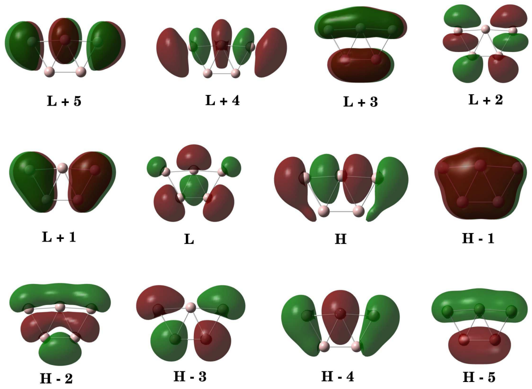

Figure 7: Molecular orbitals of pentagonal aluminum pentamer. H and L stands for HOMO and LUMO respectively.

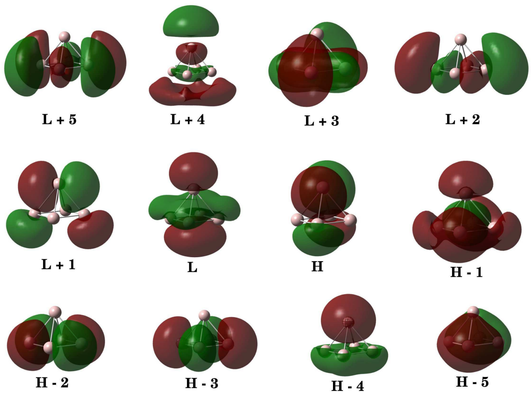

Figure 8: Molecular orbitals of pyramidal aluminum pentamer. H and L stands for HOMO and LUMO respectively.

Table I: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_2, along with the oscillator strength (f_{12}) of the transitions. Longitudinal and transverse polarization corresponds to the absorption due to light polarized along and perpendicular to the molecular axis respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1,H_2 denote SOMOs discussed earlier, and H, and L, denote HOMO and LUMO orbitals respectively. HF denotes the Hartree-Fock configuration.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[a]		$^3B_{2u}$			$\|H_1^1,\, H_2^1\rangle$ (0.9096) $\|H-1 \rightarrow H_1; H_2 \rightarrow L\rangle$(0.1139) $\|H-2 \rightarrow L; H-1 \rightarrow L+2\rangle$(0.0889)
I	1.96	$^3B_{3g}$	0.1027	longitudinal	$\|H_2 \rightarrow L+1\rangle$(0.8120) $\|H-1 \rightarrow H_1\rangle$(0.3685)
II	3.17	$^3B_{3g}$	0.1249	longitudinal	$\|H-1 \rightarrow H_1\rangle$(0.6172) $\|H_1 \rightarrow L+3\rangle$(0.4068) $\|H_1 \rightarrow L; H-1 \rightarrow L\rangle$(0.3190)
III	4.47	^3A_g	0.5149	transverse	$\|H_2 \rightarrow L+4\rangle$(0.8313) $\|H_2 \rightarrow L+6\rangle$(0.2024)
IV	4.99	$^3B_{3g}$	5.4531	longitudinal	$\|H_1 \rightarrow L+3\rangle$(0.7353) $\|H-1 \rightarrow H_1\rangle$(0.4104)
V	6.31	^3A_g	0.2554	transverse	$\|H_2 \rightarrow L+6\rangle$(0.4683) $\|H-1 \rightarrow L+1\rangle$(0.3894) $\|H-1 \rightarrow L; H_2 \rightarrow L+2\rangle$(0.3886)
VI	7.17	^3A_g	0.1549	transverse	$\|H_2 \rightarrow L+2; H-1 \rightarrow L\rangle$(0.4782) $\|H-1 \rightarrow L+1\rangle$(0.4327) $\|H_1 \rightarrow L; H_2 \rightarrow L+8\rangle$(0.3867)
VII	7.79	^3A_g	1.2530	transverse	$\|H-1 \rightarrow H_1; H_2 \rightarrow L+3\rangle$(0.4833) $\|H_1 \rightarrow L+7\rangle$(0.3917) $\|H_1 \rightarrow L; H_2 \rightarrow L+8\rangle$(0.3791)
VIII	8.05	$^3B_{1g}$	3.5391	transverse	$\|H-2 \rightarrow L\rangle$(0.5316) $\|H-1 \rightarrow L+2\rangle$(0.3756) $\|H_1 \rightarrow L+8\rangle$(0.3531)
	8.10	^3A_g	1.1418	transverse	$\|H-1 \rightarrow H_1; H_2 \rightarrow L+3\rangle$(0.4788) $\|H_2 \rightarrow L+6\rangle$(0.4095)
IX	8.87	$^3B_{1g}$	0.7044	transverse	$\|H_1 \rightarrow L+11\rangle$(0.5061) $\|H_1 \rightarrow L; H_2 \rightarrow L+7\rangle$(0.4162)
	8.95	^3A_g	0.6872	transverse	$\|H_1 \rightarrow L+7\rangle$(0.4932) $\|H_2 \rightarrow L; H_1 \rightarrow L+8\rangle$(0.4414) $\|H_1 \rightarrow L+4; H-1 \rightarrow L+1\rangle$(0.3262)

[a] GS does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_2 isomer.

Table II: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of metastable Al_2, along with the oscillator strength (f_{12}) of the transitions. Longitudinal and transverse polarization corresponds to the absorption due to light polarized along and perpendicular to the molecular axis respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1,H_2 denote SOMOs discussed earlier, and H, and L, denote HOMO and LUMO orbitals respectively. HF denotes the Hartree-Fock configuration.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[b]		$^3B_{3g}$			$\|H_1^1, H_2^1\rangle$ (0.8975) $\|H-1 \rightarrow L; H-1 \rightarrow L\rangle(0.1418)$ $\|H-1 \rightarrow L; H_1 \rightarrow L+1\rangle(0.1146)$
I	2.29	^3A_u	0.0283	longitudinal	$\|H-1 \rightarrow L\rangle(0.6598)$ $\|H_1 \rightarrow L+1\rangle(0.4276)$ $\|H_2 \rightarrow L+1\rangle(0.4276)$
II	3.26	^3A_u	0.0350	longitudinal	$\|H-1 \rightarrow L\rangle(0.7659)$ $\|H_1 \rightarrow L\rangle(0.3137)$
III	4.40	$^3B_{2u,3u}$	0.0469	transverse	$\|H-1 \rightarrow L+1\rangle(0.5540)$ $\|H_2 \rightarrow L+1; H-1 \rightarrow H_1\rangle(0.4827)$
IV	4.67	$^3B_{2u,3u}$	0.1769	transverse	$\|H_1 \rightarrow L+3\rangle(0.5073)$ $\|H-1 \rightarrow L+1\rangle(0.5030)$
V	5.17	^3A_u	5.8490	longitudinal	$\|H-1 \rightarrow L\rangle(0.7286)$ $\|H_1 \rightarrow L+1\rangle(0.3078)$
VI	5.75	$^3B_{2u,3u}$	0.1549	transverse	$\|H-1 \rightarrow H_2\rangle(0.5354)$ $\|H-1 \rightarrow L+1\rangle(0.4847)$
VII	6.24	$^3B_{2u,3u}$	0.2361	transverse	$\|H-1 \rightarrow L+1\rangle(0.5856)$ $\|H-1 \rightarrow L; H-1 \rightarrow H_1\rangle(0.3432)$
VIII	6.79	$^3B_{2u,3u}$	0.0659	transverse	$\|H_1 \rightarrow L; H_2 \rightarrow L+5\rangle(0.4766)$ $\|H_1 \rightarrow L; H-1 \rightarrow L+2\rangle(0.4333)$
IX	7.73	^3A_u	0.5428	longitudinal	$\|H-1 \rightarrow L+3\rangle(0.6484)$ $\|H_1 \rightarrow L+1; H-1 \rightarrow L\rangle(0.2333)$
X	8.13	$^3B_{2u,3u}$	3.6959	transverse	$\|H-1 \rightarrow L+1\rangle(0.4767)$ $\|H_2 \rightarrow L+4\rangle(0.4052)$
XI	8.49	$^3B_{2u,3u}$	1.1382	transverse	$\|H_1 \rightarrow L; H-1 \rightarrow L+2\rangle(0.4727)$ $\|H-2 \rightarrow H_1\rangle(0.3364)$

[b] GS does not correspond to any peak, rather it corresponds to the ground state wavefunction of metastable Al_2 isomer.

Table III: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_3 equilateral triangle isomer, along with the oscillator strength (f_{12}) of the transitions. In-plane and transverse polarization corresponds to the absorption due to light polarized in and perpendicular to the plane of the triangular isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H and L, denote HOMO (singly occupied, in this case) and LUMO orbitals respectively. HF denotes the Hartree-Fock configuration.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[c]		$^2A_1$			$\|HF\rangle$ (0.8373) $\|H-2 \rightarrow L+5\rangle$(0.1329)
I	3.42	$^2B_2$	0.0376	in-plane	$\|H-3 \rightarrow L+5\rangle$(0.2908) $\|H-2 \rightarrow L+1\rangle$(0.2439)
	3.54	$^2A_1$	0.1080	in-plane	$\|H-2 \rightarrow L+5\rangle$(0.3686) $\|H-2 \rightarrow H\rangle$(0.3403)
II	5.61	$^2A_1$	0.2565	in-plane	$\|H-2 \rightarrow L+5; H-1 \rightarrow L+5\rangle$(0.4854) $\|H \rightarrow L+1; H-1 \rightarrow L+1\rangle$(0.4476)
III	5.87	$^2B_1$	0.3413	transverse	$\|H-3 \rightarrow L+2\rangle$(0.2915) $\|H-2 \rightarrow L\rangle$(0.2842)
IV	6.53	$^2A_1$	6.3289	in-plane	$\|H \rightarrow L+6\rangle$(0.4044) $\|H-3 \rightarrow L+1\rangle$(0.3965) $\|H-2 \rightarrow L+5\rangle$(0.3158)
	6.53	$^2B_2$	5.7925	in-plane	$\|H \rightarrow L+4\rangle$(0.3842) $\|H-3 \rightarrow L+5\rangle$(0.2834) $\|H-4 \rightarrow L+1\rangle$(0.2256)
V	6.96	$^2B_1$	0.4145	transverse	$\|H-2 \rightarrow L\rangle$(0.3140) $\|H-3 \rightarrow L+2\rangle$(0.2626)
VI	7.50	$^2B_2$	0.9430	in-plane	$\|H-2 \rightarrow L+1; H \rightarrow L+5\rangle$(0.3136) $\|H-3 \rightarrow L+5\rangle$(0.2864)
	7.57	$^2A_1$	0.8630	in-plane	$\|H \rightarrow L+5; H-3 \rightarrow L+1\rangle$(0.3838) $\|H-3 \rightarrow L+1\rangle$(0.2651) $\|H-2 \rightarrow L+5\rangle$(0.2590)

[c] GS does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_3 equilateral triangle isomer.

Table IV: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_3 isosceles triangle isomer, along with the oscillator strength (f_{12}) of the transitions. In-plane and transverse polarization corresponds to the absorption due to light polarized in and perpendicular to the plane of the triangular isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1, H_2 and H_3 denote SOMOs discussed earlier, H and L, denote HOMO and LUMO orbitals respectively.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[d]		${}^4A_1$			$\lvert H_1^1, H_2^1, H_3^1\rangle$ (0.8670) $\lvert H-1 \rightarrow L+10\rangle$(0.1213)
I	2.37	${}^4A_2$	0.0358	in-plane	$\lvert H_1 \rightarrow L+1; H_3 \rightarrow L+2\rangle$(0.7066) $\lvert H-1 \rightarrow L+1; H_1 \rightarrow L\rangle$(0.4052)
II	3.06	${}^4B_1$	0.0992	in-plane	$\lvert H_3 \rightarrow H_2; H-2 \rightarrow L\rangle$(0.4691) $\lvert H-1 \rightarrow L+1; H_3 \rightarrow H_2\rangle$(0.4070)
III	3.45	${}^4A_2$	0.0967	in-plane	$\lvert H_1 \rightarrow L+3\rangle$(0.5566) $\lvert H-1 \rightarrow L+1; H_1 \rightarrow L\rangle$(0.5209)
IV	4.11	${}^4B_1$	0.3208	in-plane	$\lvert H_1 \rightarrow L+4\rangle$(0.6038) $\lvert H_3 \rightarrow L+1; H-2 \rightarrow L\rangle$(0.5272)
V	4.83	${}^4A_2$	0.2242	in-plane	$\lvert H_1 \rightarrow L+1; H-2 \rightarrow L+1\rangle$(0.5321) $\lvert H_1 \rightarrow L+5\rangle$(0.2611)
VI	5.76	${}^4A_2$	5.0792	in-plane	$\lvert H-1 \rightarrow L+1; H_3 \rightarrow L\rangle$(0.3479) $\lvert H-3 \rightarrow L+1; H_1 \rightarrow L\rangle$(0.2875) $\lvert H_2 \rightarrow L+1; H_1 \rightarrow L+3\rangle$(0.2800)
	5.85	${}^4B_1$	0.8553	in-plane	$\lvert H_3 \rightarrow L+1; H-2 \rightarrow L\rangle$(0.4081) $\lvert H-1 \rightarrow L; H_3 \rightarrow L\rangle$(0.2400)
VII	5.95	${}^4A_2$	1.7094	in-plane	$\lvert H-1 \rightarrow L+2\rangle$(0.3296) $\lvert H-1 \rightarrow L+1; H_3 \rightarrow L\rangle$(0.3138)
	6.15	${}^4B_1$	0.7827	in-plane	$\lvert H_1 \rightarrow L+7\rangle$(0.7827)
VIII	6.68	${}^4B_1$	1.7774	in-plane	$\lvert H_1 \rightarrow L+10\rangle$(0.4548) $\lvert H_2 \rightarrow L+1; H_1 \rightarrow L+6\rangle$(0.2705) $\lvert H_1 \rightarrow L+6\rangle$(0.2447)

[d] *GS* does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_3 isosceles triangle isomer.

Table V: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_3 linear isomer, along with the oscillator strength (f_{12}) of the transitions. Longitudinal and transverse polarization corresponds to the absorption due to light polarized along and perpendicular to the axis of the linear isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1, H_2 and H_3 denote SOMOs discussed earlier, H and L, denote HOMO and LUMO orbitals respectively. HF denotes the Hartree-Fock configuration.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[e]		${}^4A_u$			$\|H_1^1, H_2^1, H_3^1\rangle$ (0.8010) $\|H-3 \rightarrow H_1; H_3 \rightarrow L\rangle$(0.1913)
I	1.24	${}^4B_{3g}$	0.0317	longitudinal	$\|H_2 \rightarrow L+1\rangle$(0.6602) $\|H-1 \rightarrow H_3\rangle$(0.3636)
II	2.25	${}^4B_{3g}$	0.0489	longitudinal	$\|H-1 \rightarrow H_3\rangle$(0.6856) $\|H-2 \rightarrow H_1\rangle$(0.3230)
III	4.01	${}^4B_{3g}$	0.9019	longitudinal	$\|H-2 \rightarrow H_1\rangle$(0.5249) $\|H-1 \rightarrow H_3\rangle$(0.3471)
IV	4.43	${}^4B_{3g}$	2.8593	longitudinal	$\|H-1 \rightarrow H_3\rangle$(0.4070) $\|H-1 \rightarrow L+4; H_2 \rightarrow L+6\rangle$(0.2409)
	4.47	${}^4B_{1g,2g}$	0.0960	transverse	$\|H_2 \rightarrow L+2\rangle$(0.5402) $\|H-1 \rightarrow H_3; H_2 \rightarrow L+6\rangle$(0.3068)
V	4.62	${}^4B_{3g}$	5.1747	longitudinal	$\|H-1 \rightarrow H_3\rangle$(0.4600) $\|H-1 \rightarrow L+4; H_2 \rightarrow L+6\rangle$(0.2862)
VI	5.29	${}^4B_{1g,2g}$	0.1070	transverse	$\|H_2 \rightarrow L+5\rangle$(0.4951) $\|H-1 \rightarrow H_3; H-1 \rightarrow L+1\rangle$(0.3284) $\|H-1 \rightarrow L+3\rangle$(0.3091)
VII	5.83	${}^4B_{3g}$	0.1412	longitudinal	$\|H-1 \rightarrow L+2; H_1 \rightarrow L\rangle$(0.6637) $\|H-2 \rightarrow H_1\rangle$(0.2225) $\|H-1 \rightarrow H_3\rangle$(0.2073)
VIII	6.31	${}^4B_{3g}$	0.0459	longitudinal	$\|H_1 \rightarrow L+6; H_3 \rightarrow L\rangle$(0.5099) $\|H_1 \rightarrow L; H_3 \rightarrow L+6\rangle$(0.2706)
	6.37	${}^4B_{1g,2g}$	0.0740	transverse	$\|H-1 \rightarrow L+3\rangle$(0.3989) $\|H-1 \rightarrow H_2; H_3 \rightarrow L+6\rangle$(0.2266)
IX	6.89	${}^4B_{3g}$	0.1311	longitudinal	$\|H-5 \rightarrow L+6\rangle$(0.3920) $\|H_1 \rightarrow L+4; H_3 \rightarrow L+6\rangle$(0.3086)

[e] GS does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_3 linear triangle isomer.

Table VI: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_4 rhombus isomer, along with the oscillator strength (f_{12}) of the transitions. In-plane and transverse polarization corresponds to the absorption due to light polarized in and perpendicular to the plane of the rhombus isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1,H_2 denote SOMOs discussed earlier, and H, and L, denote HOMO and LUMO orbitals respectively.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[f]		$^3B_{2g}$			$\|H_1^1, H_2^1\rangle$ (0.8724) $\|H-3 \rightarrow L; H-3 \rightarrow L\rangle$(0.1050)
I	1.07	$^3B_{1u}$	0.0247	transverse	$\|H_1 \rightarrow L+1\rangle$(0.8489) $\|H-2 \rightarrow L+5\rangle$(0.1601)
II	2.31	$^3B_{3u}$	0.3087	in-plane	$\|H-2 \rightarrow H_1\rangle$(0.7645) $\|H_2 \rightarrow L+1\rangle$(0.3113)
III	4.67	$^3B_{3u}$	0.5709	in-plane	$\|H-2 \rightarrow L; H-1 \rightarrow L+3\rangle$(0.6036) $\|H-1 \rightarrow L+3\rangle$(0.4213) $\|H_1 \rightarrow L+7\rangle$(0.3113)
IV	4.88	^3A_u	0.9622	in-plane	$\|H-1 \rightarrow L; H-1 \rightarrow L+3\rangle$(0.6036) $\|H-3 \rightarrow L\rangle$(0.4699)
V	5.51	$^3B_{3u}$	3.8316	in-plane	$\|H-3 \rightarrow L+4\rangle$(0.7378) $\|H-2 \rightarrow H_1\rangle$(0.2161)
VI	5.84	^3A_u	0.4900	in-plane	$\|H-2 \rightarrow L+3\rangle$(0.3889) $\|H-2 \rightarrow L; H-3 \rightarrow L\rangle$(0.3758) $\|H-3 \rightarrow L\rangle$(0.3594) $\|H-1 \rightarrow L; H-1 \rightarrow L+3\rangle$(0.3591)
VII	6.01	$^3B_{1u}$	0.5332	transverse	$\|H_2 \rightarrow L+7\rangle$(0.7268) $\|H-3 \rightarrow L+2\rangle$(0.3050)
VIII	6.20	^3A_u	0.7477	in-plane	$\|H-2 \rightarrow L+3\rangle$(0.5195) $\|H-2 \rightarrow L; H-3 \rightarrow L\rangle$(0.4189)
IX	6.51	$^3B_{1u}$	0.2928	transverse	$\|H-3 \rightarrow L+2\rangle$(0.7001) $\|H-2 \rightarrow H_1; H-1 \rightarrow L+2\rangle$(0.2232) $\|H-2 \rightarrow L; H-3 \rightarrow L+2\rangle$(0.2070)
X	6.92	$^3B_{1u}$	0.6053	transverse	$\|H-3 \rightarrow L+2\rangle$(0.5144) $\|H-2 \rightarrow L; H-3 \rightarrow L+2\rangle$(0.3549) $\|H-2 \rightarrow L+5\rangle$(0.2676)
XI	7.31	$^3B_{1u}$	0.4328	transverse	$\|H-2 \rightarrow L+5\rangle$(0.4033) $\|H-3 \rightarrow L; H-1 \rightarrow L+1\rangle$(0.3787)
XII	7.76	$^3B_{3u}$	2.7450	in-plane	$\|H_1 \rightarrow L+8\rangle$(0.4387) $\|H_1 \rightarrow L+1; H-1 \rightarrow L+2\rangle$(0.3435)

[f] GS does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_4 rhombus isomer.

Table VII: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_4 square isomer, along with the oscillator strength (f_{12}) of the transitions. In-plane and transverse polarization corresponds to the absorption due to light polarized in and perpendicular to the plane of the rhombus isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H_1,H_2 denote SOMOs discussed earlier, and H, and L, denote HOMO and LUMO orbitals respectively.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[g]		$^3B_{3u}$			$\vert H_1^1, H_2^1\rangle(0.8525)$ $\vert H_1 \rightarrow L; H-2 \rightarrow L\rangle(0.0972)$
I	2.08	$^3B_{1g,2g}$	0.0278	in-plane	$\vert H-1 \rightarrow L\rangle(0.7191)$ $\vert H-1 \rightarrow H_1; H_2 \rightarrow L+1\rangle(0.2645)$ $\vert H_2 \rightarrow L+1\rangle(0.2536)$ $\vert H_1 \rightarrow L\rangle(0.2443)$
II	2.68	$^3B_{1g,2g}$	0.0301	in-plane	$\vert H_2 \rightarrow L+1\rangle(0.4757)$ $\vert H-1 \rightarrow L\rangle(0.4358)$ $\vert H-1 \rightarrow H_1; H_2 \rightarrow L+1\rangle(0.3608)$
III	4.19	$^3B_{1g,2g}$	0.3420	in-plane	$\vert H-2 \rightarrow L\rangle(0.5889)$ $\vert H-1 \rightarrow L+2\rangle(0.4283)$ $\vert H_1 \rightarrow L\rangle(0.2329)$
IV	4.92	$^3B_{1g,2g}$	0.1131	in-plane	$\vert H_1 \rightarrow L+2\rangle(0.5780)$ $\vert H-1 \rightarrow L+2\rangle(0.4083)$ $\vert H-2 \rightarrow L\rangle(0.3198)$
V	5.17	^3A_g	0.1238	transverse	$\vert H-2 \rightarrow L; H_1 \rightarrow L+1\rangle(0.3693)$ $\vert H-2 \rightarrow L; H_1 \rightarrow L+1\rangle(0.3692)$
	5.33	$^3B_{1g,2g}$	0.2470	in-plane	$\vert H-2 \rightarrow H_1; H-2 \rightarrow L\rangle(0.5193)$ $\vert H-1 \rightarrow L+2\rangle(0.3915)$ $\vert H-2 \rightarrow L+2\rangle(0.3335)$
VI	5.85	$^3B_{1g,2g}$	1.2446	in-plane	$\vert H-2 \rightarrow L+2\rangle(0.7184)$ $\vert H-1 \rightarrow H_1; H-2 \rightarrow L+2\rangle(0.2587)$ $\vert H-1 \rightarrow L+2\rangle(0.2579)$
VII	6.55	$^3B_{1g,2g}$	3.7894	in-plane	$\vert H-2 \rightarrow L+2\rangle(0.5706)$ $\vert H-1 \rightarrow H_1; H-2 \rightarrow L+2\rangle(0.4089)$ $\vert H-1 \rightarrow L+2\rangle(0.3325)$
	6.58	^3A_g	0.2634	transverse	$\vert H_1 \rightarrow L+1; H-2 \rightarrow L\rangle(0.4375)$ $\vert H_1 \rightarrow L+1; H-2 \rightarrow L\rangle(0.4375)$ $\vert H-2 \rightarrow L+3\rangle(0.4183)$
VIII	6.87	$^3B_{1g,2g}$	2.9702	in-plane	$\vert H-2 \rightarrow L+2\rangle(0.5100)$ $\vert H-1 \rightarrow L+2\rangle(0.3495)$
	6.93	^3A_g	0.2483	transverse	$\vert H_1 \rightarrow L+1; H-2 \rightarrow L\rangle(0.3558)$ $\vert H_1 \rightarrow L+1; H-2 \rightarrow L\rangle(0.3558)$ $\vert H-2 \rightarrow L+3\rangle(0.2929)$
IX	7.22	$^3B_{1g,2g}$	1.4267	in-plane	$\vert H-1 \rightarrow H_1; H-2 \rightarrow L+2\rangle(0.4039)$ $\vert H-3 \rightarrow H_1\rangle(0.2900)$ $\vert H-1 \rightarrow H_1; H-1 \rightarrow L+2\rangle(0.2848)$

[g] *GS* does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_4 square isomer.

Table VIII: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_5 pentagonal isomer, along with the oscillator strength (f_{12}) of the transitions. In-plane and transverse polarization corresponds to the absorption due to light polarized in and perpendicular to the plane of the pentagonal isomer respectively. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H and L, denote HOMO and LUMO orbitals respectively.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[h]		$^2A_1$			$\vert(H-2)^1\rangle$ (0.8679) $\vert H-2 \rightarrow L+1; H \rightarrow L+2\rangle$(0.1045)
I	1.03	$^2B_2$	0.0195	in-plane	$\vert H-1 \rightarrow L\rangle$(0.8635) $\vert H-1 \rightarrow L; H \rightarrow L+3\rangle$(0.0880)
II	2.38	$^2B_2$	0.0219	in-plane	$\vert H-3 \rightarrow H-2\rangle$(0.8560) $\vert H-1 \rightarrow L+4\rangle$(0.1387)
III	3.90	$^2B_1$	0.1042	transverse	$\vert H \rightarrow L+4\rangle$(0.8387) $\vert H \rightarrow L; H-1 \rightarrow L+2\rangle$(0.1944)
		$^2A_1$	0.3362	in-plane	$\vert H-4 \rightarrow L\rangle$(0.8140) $\vert H-2 \rightarrow L+9\rangle$(0.1841)
IV	4.16	$^2B_2$	1.3144	in-plane	$\vert H-1 \rightarrow L+4\rangle$(0.7276) $\vert H-1 \rightarrow L+5\rangle$(0.4478)
V	4.42	$^2B_2$	3.3339	in-plane	$\vert H-1 \rightarrow L+5\rangle$(0.7096) $\vert H-1 \rightarrow L+4\rangle$(0.4490) $\vert H-1 \rightarrow L+9\rangle$(0.1535)
VI	4.78	$^2A_1$	1.0471	in-plane	$\vert H-2 \rightarrow L+9\rangle$(0.7992) $\vert H-2 \rightarrow L; H \rightarrow L+6\rangle$(0.2058)
VII	5.46	$^2B_1$	1.1014	transverse	$\vert H \rightarrow L+13\rangle$(0.8156) $\vert H \rightarrow L; H-2 \rightarrow L\rangle$(0.1708)
VIII	6.37	$^2B_2$	0.1270	in-plane	$\vert H-3 \rightarrow L\rangle$(0.7632)
IX	6.73	$^2B_2$	0.7104	in-plane	$\vert H-3 \rightarrow L\rangle$(0.7370) $\vert H \rightarrow L+1\rangle$(0.3698) $\vert H-1 \rightarrow L; H \rightarrow L+3\rangle$(0.1225)
X	7.49	$^2A_1$	0.3989	in-plane	$\vert H \rightarrow L+3\rangle$(0.5087) $\vert H-2 \rightarrow L+16\rangle$(0.3508) $\vert H \rightarrow L; H-1 \rightarrow L+1\rangle$(0.2937)

[h] *GS* does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_5 pentagonal isomer.

Table IX: Excitation energies (E) and many-particle wave functions of excited states corresponding to the peaks in the linear absorption spectrum of Al_5 pyramid isomer, along with the oscillator strength (f_{12}) of the transitions. In the wave function, the bracketed numbers are the CI coefficients of a given electronic configuration. Symbols H and L, denote HOMO and LUMO orbitals respectively.

Peak	E (eV)	Symmetry	f_{12}	Polarization	Wave Function
GS[i]		$^2A_1$			$\lvert (H-2)^1 \rangle$ (0.8591) $\lvert H-3 \rightarrow L+1; H-3 \rightarrow L+1 \rangle$(0.1138)
I	1.72	$^2B_2$	0.0046	y	$\lvert H-3 \rightarrow L+1 \rangle$(0.6849) $\lvert H-2 \rightarrow L+1 \rangle$(0.2887)
	1.75	$^2A_1$	0.0521	z	$\lvert H \rightarrow L+3 \rangle$(0.2887)
II	2.21	$^2B_2$	0.0296	y	$\lvert H-3 \rightarrow L+1 \rangle$(0.7170) $\lvert H-2 \rightarrow L+2 \rangle$(0.3402) $\lvert H-3 \rightarrow L+2 \rangle$(0.2290)
III	2.55	$^2A_1$	0.0477	z	$\lvert H \rightarrow L+3 \rangle$(0.5390) $\lvert H-4 \rightarrow H-2 \rangle$(0.1296)
IV	3.46	$^2B_2$	0.0399	y	$\lvert H-3 \rightarrow L; H-2 \rightarrow L+1 \rangle$(0.6131) $\lvert H-3 \rightarrow L+2 \rangle$(0.4975)
	3.48	$^2A_1$	0.0769	z	$\lvert H-4 \rightarrow H-2 \rangle$(0.7340) $\lvert H-4 \rightarrow L \rangle$(0.3735)
V	4.04	$^2B_1$	0.6432	x	$\lvert H \rightarrow L+7 \rangle$(0.5929) $\lvert H \rightarrow L+4 \rangle$(0.4432)
	4.22	$^2B_2$	3.0735	y	$\lvert H-3 \rightarrow L+2 \rangle$(0.8272) $\lvert H-3 \rightarrow L+1 \rangle$(0.1580)
VI	4.74	$^2B_1$	0.3474	x	$\lvert H \rightarrow L \rangle$(0.7617) $\lvert H \rightarrow L+7 \rangle$(0.2542)
VII	5.08	$^2A_1$	0.5494	z	$\lvert H-2 \rightarrow L; H \rightarrow L+2 \rangle$(0.5540) $\lvert H-4 \rightarrow L \rangle$(0.4833)
VIII	5.26	$^2A_1$	0.3175	z	$\lvert H-2 \rightarrow L; H \rightarrow L+5 \rangle$(0.6251) $\lvert H-4 \rightarrow L \rangle$(0.3902)
	5.27	$^2B_1$	0.1267	x	$\lvert H-6 \rightarrow H-2; H \rightarrow L+1 \rangle$(0.6056) $\lvert H \rightarrow L \rangle$(0.3242)
IX	5.56	$^2B_1$	0.1384	x	$\lvert H \rightarrow L+11 \rangle$(0.7819) $\lvert H \rightarrow L+13 \rangle$(0.3051)
X	6.00	$^2B_1$	1.0052	x	$\lvert H \rightarrow L+13 \rangle$(0.8132) $\lvert H \rightarrow L+11 \rangle$(0.1852)

[i] *GS* does not correspond to any peak, rather it corresponds to the ground state wavefunction of Al_5 pyramid isomer.