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

Probing the Low-Energy Structures of Aluminum-Magnesium Alloy Clusters: A Detailed Study

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Table S1 The electronic states, symmetries, averaged binding energy (E_b, eV), and HOMO – LUMO energy gap (E_{gap}, eV) for the lowest-energy structures of neutral and anionic Al_n (n = 3-20) clusters.

Cluster	State	Symm.	E_b	E_{gap}	Cluster	State	Symm.	E_b	E_{gap}
Al_3	$^2A_1'$	D_{3h}	0.72	1.63	Al_3^-	$^1A_1'$	D_{3h}	1.10	1.57
Al_4	^1A_g	C_{2h}	1.08	1.16	Al_4^-	^2A_g	C_{2h}	1.59	1.52
Al_5	$^2B_2$	C_{2v}	1.62	1.86	Al_5^-	$^1A_1$	C_{2v}	2.08	1.35
Al_6	^1A_g	C_{2h}	1.81	1.64	Al_6^-	^2A_g	C_{2h}	2.26	1.39
Al_7	$^2A_1$	C_{3v}	2.03	1.80	Al_7^-	$^1A_1$	C_{3v}	2.36	1.61
Al_8	^1A_g	C_{2h}	2.06	1.86	Al_8^-	^2B_u	C_{2h}	2.34	1.39
Al_9	$^2A'$	C_s	2.11	1.61	Al_9^-	^1A	C_2	2.42	1.50
Al_{10}	$^1A'$	C_s	2.17	1.53	Al_{10}^-	$^2A'$	C_s	2.44	1.50
Al_{11}	^2A	C_1	2.22	1.81	Al_{11}^-	$^1A'$	C_s	2.48	1.79
Al_{12}	$^1A_1$	C_{2v}	2.28	2.00	Al_{12}^-	$^2A'$	C_s	2.51	1.19
Al_{13}	^2A	C_1	2.37	2.60	Al_{13}^-	^1A_g	I_h	2.64	2.74
Al_{14}	^1A	C_2	2.40	1.61	Al_{14}^-	^2B	C_2	2.59	1.34
Al_{15}	$^2B_{3u}$	D_{2h}	2.41	0.29	Al_{15}^-	^1A_g	D_{2h}	2.59	1.66
Al_{16}	$^1A'$	C_s	2.43	1.60	Al_{16}^-	$^2A'$	C_s	2.61	1.48
Al_{17}	$^2B_{2u}$	D_{2h}	2.45	1.19	Al_{17}^-	^1A_g	D_{2h}	2.62	1.40
Al_{18}	$^1A'$	C_s	2.46	1.62	Al_{18}^-	^2A	C_1	2.60	1.01
Al_{19}	^2A	C_1	2.44	0.97	Al_{19}^-	^1A	C_1	2.59	1.23
Al_{20}	^1A	C_1	2.50	1.55	Al_{20}^-	^2A	C_1	2.64	1.55

Table S2 The electronic states, symmetries, averaged binding energy (E_b, eV), and HOMO – LUMO energy gap (E_{gap}, eV) for the lowest-energy structures of neutral and anionic Al_nMg (n = 3-20) clusters.

Cluster	State	Symm.	E_b	E_{gap}	Cluster	State	Symm.	E_b	E_{gap}
Al_3Mg	$^2A''$	C_s	1.09	1.56	Al_3Mg^-	$^3A_1$	C_{3v}	1.52	1.42
Al_4Mg	$^1A_1$	C_{4v}	1.38	1.81	Al_4Mg^-	^2A	C_2	1.61	1.44
Al_5Mg	$^2A''$	C_s	1.52	1.70	Al_5Mg^-	$^1A'$	C_s	1.91	1.47
Al_6Mg	$^1A_1$	C_{3v}	1.85	2.60	Al_6Mg^-	$^2A'$	C_s	2.12	1.38
Al_7Mg	$^2A''$	C_s	1.87	1.56	Al_7Mg^-	$^1A'$	C_1	2.13	1.55
Al_8Mg	$^3A''$	C_s	1.94	1.67	Al_8Mg^-	^2A	C_1	2.22	1.49
Al_9Mg	$^2A''$	C_s	2.01	1.41	Al_9Mg^-	$^1A'$	C_s	2.27	1.41
$Al_{10}Mg$	$^1A'$	C_s	2.06	1.51	$Al_{10}Mg^-$	^2A	C_1	2.30	1.24
$Al_{11}Mg$	$^2A'$	C_s	2.13	1.31	$Al_{11}Mg^-$	^1A	C_1	2.37	1.85
$Al_{12}Mg$	$^1A_1$	C_{5v}	2.20	1.19	$Al_{12}Mg^-$	$^2A_1$	C_{5v}	2.46	1.52
$Al_{13}Mg$	$^2A'$	C_s	2.31	1.58	$Al_{13}Mg^-$	$^1A'$	C_s	2.49	1.61
$Al_{14}Mg$	$^1A'$	C_s	2.31	1.79	$Al_{14}Mg^-$	$^2A'$	C_s	2.48	1.54
$Al_{15}Mg$	$^2A'$	C_s	2.32	1.43	$Al_{15}Mg^-$	$^1A'$	C_s	2.50	1.62
$Al_{16}Mg$	$^1A'$	C_s	2.36	1.35	$Al_{16}Mg^-$	$^2A'$	C_s	2.53	1.38
$Al_{17}Mg$	^2A	C_1	2.35	1.15	$Al_{17}Mg^-$	^1A	C_1	2.51	1.61
$Al_{18}Mg$	^1A	C_1	2.36	1.75	$Al_{18}Mg^-$	$^2A'$	C_s	2.50	1.41
$Al_{19}Mg$	^2A	C_1	2.41	1.36	$Al_{19}Mg^-$	^1A	C_1	2.56	1.85
$Al_{20}Mg$	^1A	C_1	2.40	1.20	$Al_{20}Mg^-$	^2A	C_1	2.54	1.29

Table S3 Electron Density ($\rho(r_{BCP})$), Laplacian ($\nabla^2\rho(r_{BCP})$), Bond Ellipticity (ε), and Curvature λ_3 at Bond Critical Points (BCP) for Mg-Al bond in the lowest-energy Al_nMg (n = 3-20) clusters.

		ρ / a.u.	$\nabla^2\rho$ / a.u.	ε	λ_3 / a.u.
Al_3Mg	Mg4-Al1	0.042	-0.025	0.376	0.010
Al_4Mg	Mg5-Al1	0.025	0.002	**3.081**	0.006
	Mg5-Al2	0.025	0.002	**3.081**	0.006
Al_5Mg	Mg1-Al3	0.024	0.013	**1.001**	0.022
	Mg1-Al5	0.024	0.013	**1.001**	0.022
Al_6Mg	Mg7-Al2	0.025	0.019	0.148	0.037
	Mg7-Al4	0.025	0.019	0.148	0.037
	Mg7-Al5	0.025	0.019	0.148	0.037
Al_7Mg	Mg8-Al6	0.024	0.030	0.194	0.043
	Mg8-Al7	0.025	0.024	0.250	0.037
Al_8Mg	Mg1-Al2	0.023	0.023	**3.128**	0.031
	Mg1-Al3	0.023	0.023	**3.128**	0.031
	Mg1-Al5	0.023	0.027	**1.795**	0.036
	Mg1-Al4	0.026	0.028	0.170	0.046
Al_9Mg	Mg1-Al2	0.024	0.023	0.726	0.036
	Mg1-Al3	0.024	0.023	0.726	0.036
	Mg1-Al4	0.027	0.027	0.197	0.050
$Al_{10}Mg$	Mg1-Al2	0.024	0.026	**1.209**	0.033
	Mg1-Al3	0.025	0.026	0.542	0.043
	Mg1-Al4	0.025	0.028	0.531	0.038
	Mg1-Al5	0.025	0.026	0.542	0.043
$Al_{11}Mg$	Mg12-Al2	0.023	0.027	0.660	0.032
	Mg12-Al4	0.023	0.021	**1.412**	0.026
	Mg12-Al6	0.023	0.023	**2.021**	0.031
	Mg12-Al7	0.023	0.023	**2.021**	0.031
	Mg12-Al10	0.023	0.021	**1.412**	0.026
$Al_{12}Mg$	Mg2-Al1	0.030	0.055	0.000	0.072
$Al_{13}Mg$	Mg14-Al5	0.024	0.032	0.590	0.045
	Mg14-Al6	0.023	0.024	0.307	0.032
	Mg14-Al8	0.023	0.033	**1.819**	0.039
	Mg14-Al13	0.022	0.024	0.307	0.032
$Al_{14}Mg$	Mg15-Al12	0.023	0.032	0.079	0.037
$Al_{15}Mg$	Mg16-Al4	0.023	0.031	0.140	0.045
	Mg16-Al7	0.022	0.017	0.000	0.027
$Al_{16}Mg$	Mg17-Al14	0.021	0.022	**1.404**	0.025
	Mg17-Al15	0.022	0.032	0.754	0.039
	Mg17-Al16	0.019	0.017	0.135	0.029
$Al_{17}Mg$	Mg18-Al12	0.024	0.029	0.167	0.051
	Mg18-Al17	0.026	0.031	0.077	0.056
	Mg18-Al13	0.026	0.031	0.083	0.058

$Al_{18}Mg$	Mg19-Al6	0.020	0.025	**3.494**	0.032
	Mg19-Al11	0.021	0.013	**1.839**	0.018
$Al_{19}Mg$	Mg20-Al4	0.021	0.025	**5.011**	0.033
	Mg20-Al5	0.021	0.025	**5.194**	0.033
	Mg20-Al11	0.022	0.020	**2.583**	0.030
	Mg20-Al12	0.022	0.020	**2.561**	0.030
$Al_{20}Mg$	Mg21-Al12	0.021	0.020	**6.452**	0.030
	Mg21-Al15	0.021	0.021	**7.193**	0.031
	Mg21-Al11	0.025	0.023	0.272	0.045
	Mg21-Al20	0.022	0.026	**8.654**	0.038

Table S4 Electron Density ($\rho(r_{BCP})$), Laplacian ($\nabla^2\rho(r_{BCP})$), Bond Ellipticity (ε), and Curvature λ_3 at Bond Critical Points (BCP) for Mg-Al bond in the lowest-energy Al_nMg^- (n = 3-20) clusters.

		ρ / a.u.	$\nabla^2\rho$ / a.u.	ε	λ_3 / a.u.
Al_3Mg^-	Mg4-Al3	0.026	0.011	0.000	0.018
Al_4Mg^-	Mg5-Al1	0.025	0.018	**1.276**	0.028
	Mg5-Al3	0.025	0.018	**1.276**	0.028
Al_5Mg^-	Mg6-Al1	0.023	0.013	0.705	0.023
	Mg6-Al3	0.023	0.013	0.705	0.023
Al_6Mg^-	Mg7-Al2	0.024	0.020	0.570	0.033
	Mg7-Al4	0.024	0.020	0.570	0.033
	Mg7-Al5	0.025	0.022	0.208	0.041
Al_7Mg^-	Mg1-Al2	0.026	0.026	0.182	0.049
	Mg1-Al3	0.026	0.026	0.182	0.049
Al_8Mg^-	Mg1-Al4	0.026	0.029	0.002	0.047
	Mg1-Al5	0.024	0.029	0.937	0.040
Al_9Mg^-	Mg1-Al2	0.026	0.032	0.232	0.053
	Mg1-Al3	0.026	0.032	0.232	0.053
	Mg1-Al4	0.024	0.025	0.225	0.040
$Al_{10}Mg^-$	Mg1-Al3	0.024	0.024	0.506	0.042
	Mg1-Al4	0.021	0.020	**12.900**	0.023
	Mg1-Al5	0.023	0.023	0.567	0.040
$Al_{11}Mg^-$	Mg1-Al2	0.026	0.024	0.247	0.049
	Mg1-Al5	0.026	0.031	0.146	0.052
$Al_{12}Mg^-$	Mg2-Al1	0.026	0.044	0.000	0.055
$Al_{13}Mg^-$	Mg14-Al5	0.024	0.034	**1.633**	0.045
	Mg14-Al8	0.024	0.037	0.669	0.046
$Al_{14}Mg^-$	Mg15-Al12	0.023	0.034	0.175	0.041
$Al_{15}Mg^-$	Mg16-Al14	0.024	0.031	0.153	0.048
	Mg16-Al9	0.022	0.020	**1.854**	0.028
	Mg16-Al10	0.022	0.020	**1.854**	0.028
$Al_{16}Mg^-$	Mg17-Al15	0.022	0.035	0.283	0.041
	Mg17-Al16	0.020	0.012	0.772	0.017
$Al_{17}Mg^-$	Mg18-Al2	0.024	0.029	0.175	0.051
	Mg18-Al7	0.026	0.030	0.119	0.054
	Mg18-Al13	0.025	0.031	0.135	0.055
$Al_{18}Mg^-$	Mg19-Al6	0.021	0.025	0.558	0.035
	Mg19-Al11	0.023	0.021	0.140	0.041
	Mg19-Al18	0.021	0.025	0.558	0.035
$Al_{19}Mg^-$	Mg20-Al11	0.022	0.022	**1.352**	0.034
	Mg20-Al16	0.020	0.024	**2.892**	0.033
	Mg20-Al19	0.021	0.024	**8.405**	0.033
$Al_{20}Mg^-$	Mg21-Al12	0.022	0.023	**1.790**	0.037
	Mg21-Al11	0.024	0.019	0.267	0.039

Mg21-Al20	0.023	0.031	**1.944**	0.046

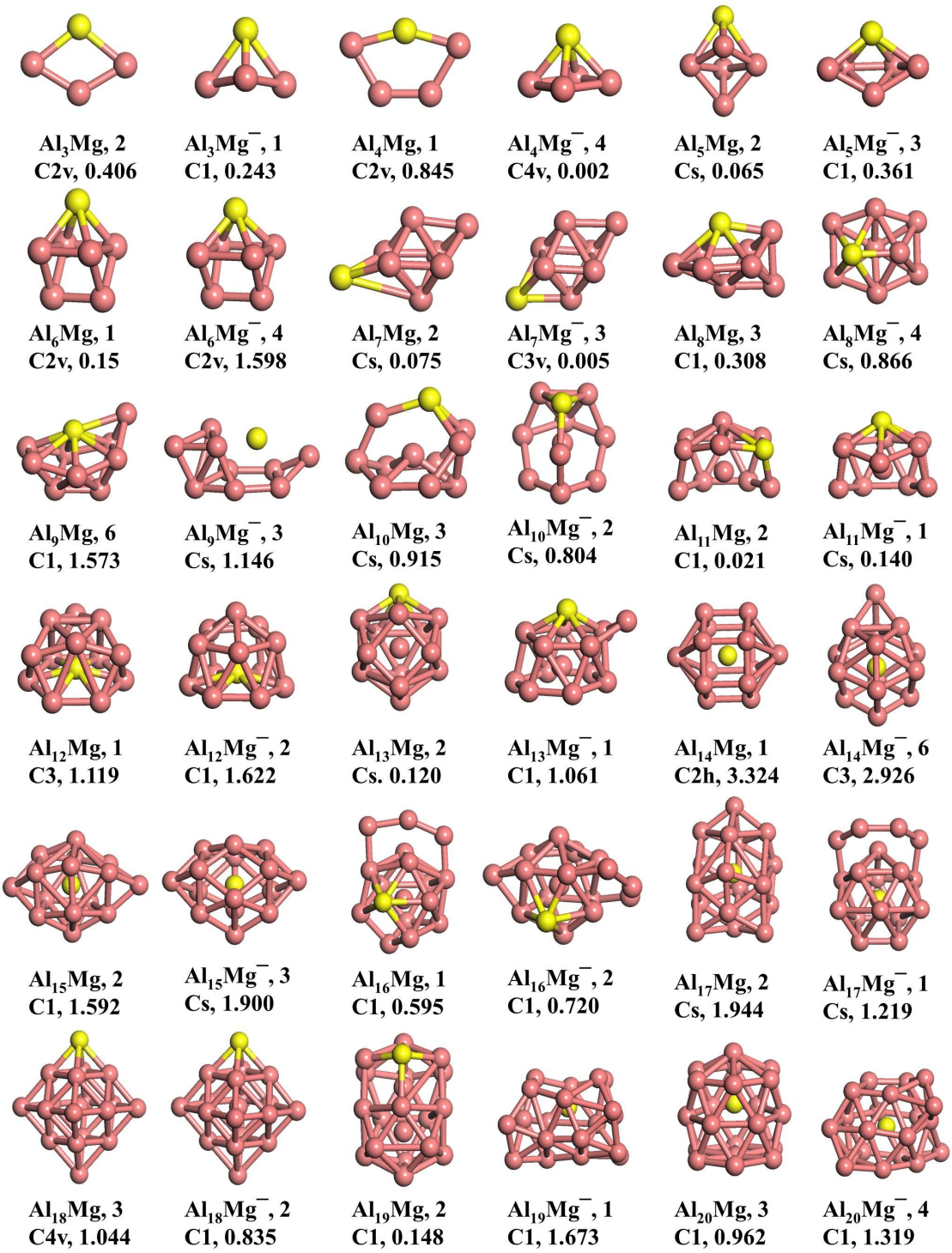

Fig S1 The metastable isomers of neutral and anionic Al_nMg (n = 4-20) clusters, together with spin multiplicity, point symmetry and relative energies.