Electronic Supplementary Information (ESI) available for:

Evolution of the structural and electronic properties of beryllium-doped aluminum clusters: comparison with neutral and cationic aluminum clusters

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Table S1. Binding energy per atom (E_b, in eV), the second difference in energy (Δ^2E, in eV), and the dissociation energy (ΔE, in eV) of the most stable Al_nBe (n = 1–13) clusters.

clusters	E_b		ΔE		Δ^2E	
	CCSD(T)	B3LYP	CCSD(T)	B3LYP	CCSD(T)	B3LYP
AlBe	0.141	0.308	-0.281	-0.616		
Al_2Be	0.622	0.822	-1.584	-1.849	-0.424	-0.333
Al_3Be	0.968	1.162	-2.008	-2.182	-0.017	-0.036
Al_4Be	1.179	1.373	-2.024	-2.217	0.178	0.163
Al_5Be	1.290	1.486	-1.846	-2.054	-1.581	-1.396
Al_6Be	1.596	1.767	-3.427	-3.450	2.093	1.975
Al_7Be	1.563	1.731	-1.334	-1.476	-0.822	-0.662
Al_8Be	1.629	1.776	-2.156	-2.138	-0.038	-0.168
Al_9Be	1.685	1.829	-2.194	-2.306	0.012	-0.053
$Al_{10}Be$	1.731	1.877	-2.182	-2.359	-0.414	-0.096
$Al_{11}Be$	1.803	1.925	-2.595	-2.454	-0.667	-0.757
$Al_{12}Be$	1.915	2.024	-3.263	-3.211	0.498	0.563
$Al_{13}Be$	1.976	2.069	-2.765	-2.648		

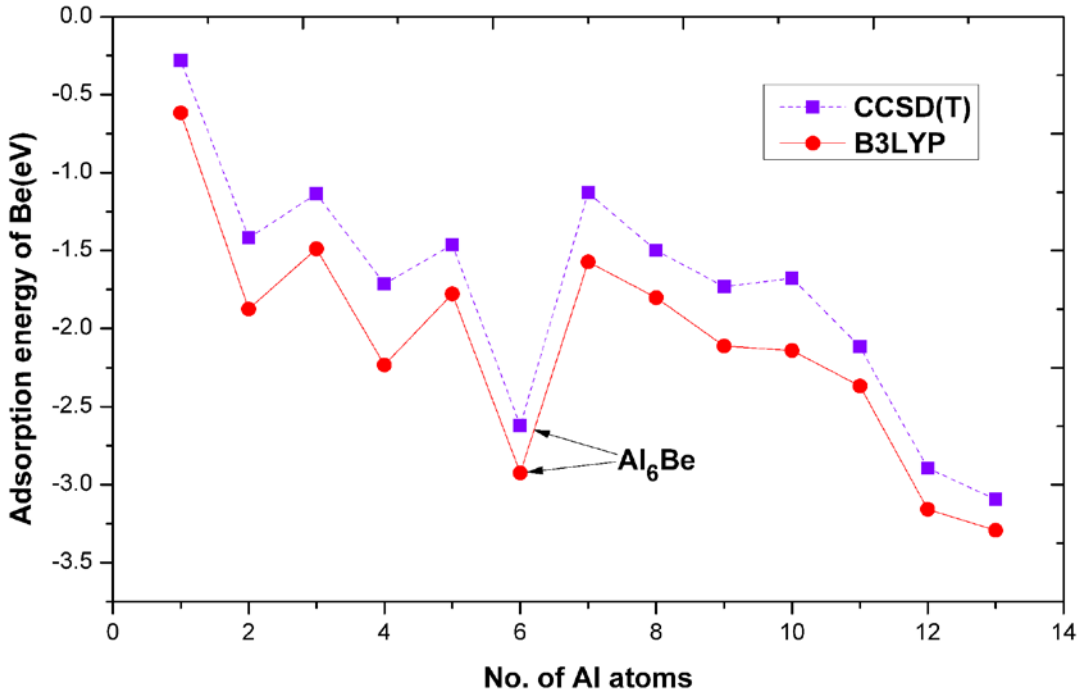

Figure S1. The adsorption energies of Be (E_{ad}) (in eV) for the lowest-energy structures of Al_nBe clusters with $1 \leq n \leq 13$ at the CCSD(T)/aug-cc-pVDZ (dashed line) and B3LYP/aug-cc-pVDZ (solid line) levels, shown as a function of the number of Al atoms.

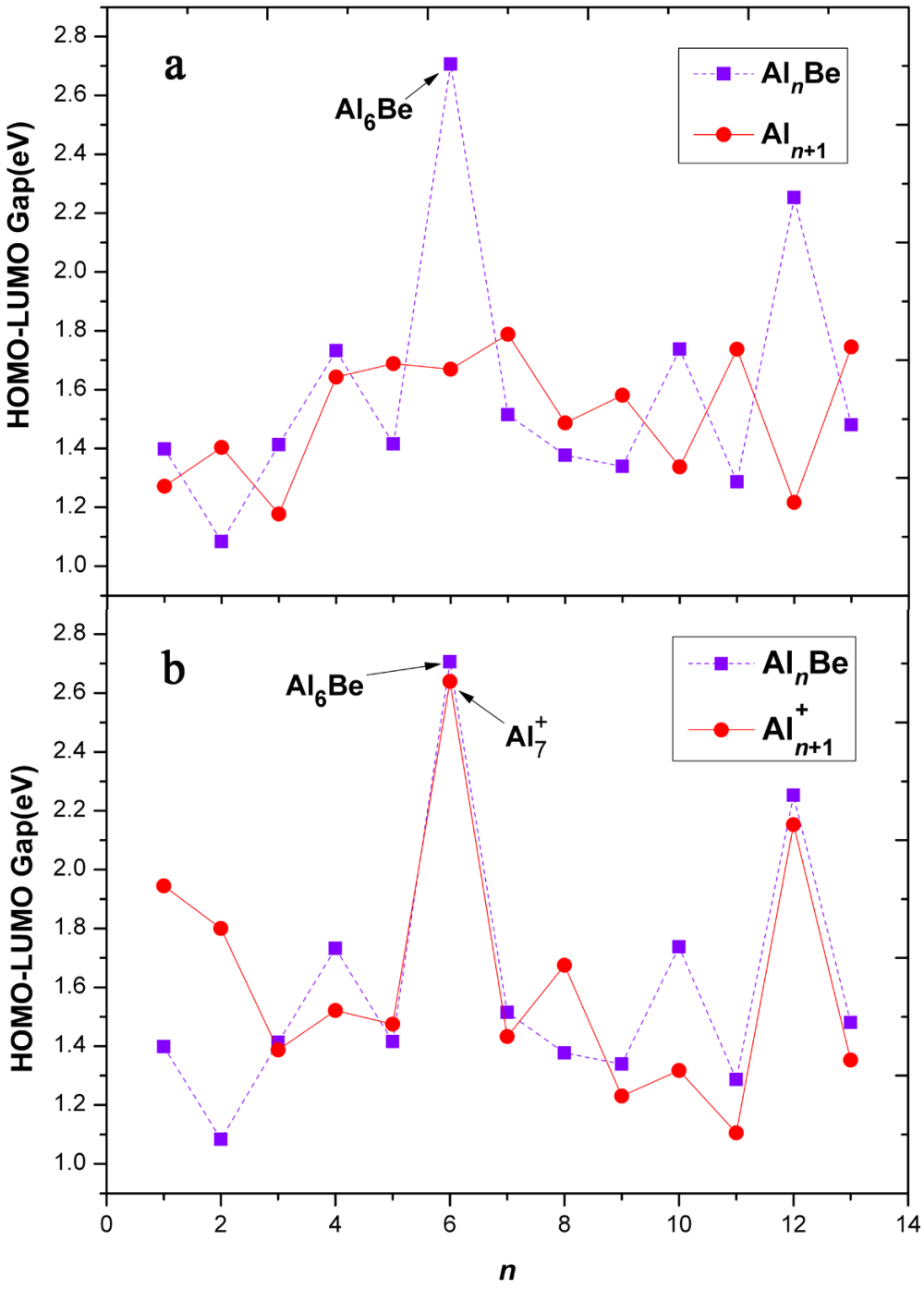

Figure S2. The HOMO–LUMO energy gaps (in eV) for the lowest-energy structures of Al_nBe (dashed line) and (a) Al_{n+1} clusters (solid line) and (b) Al_{n+1}^+ cluster cations (solid line) at the B3LYP/aug-cc-pVDZ level, shown as a function of *n*.

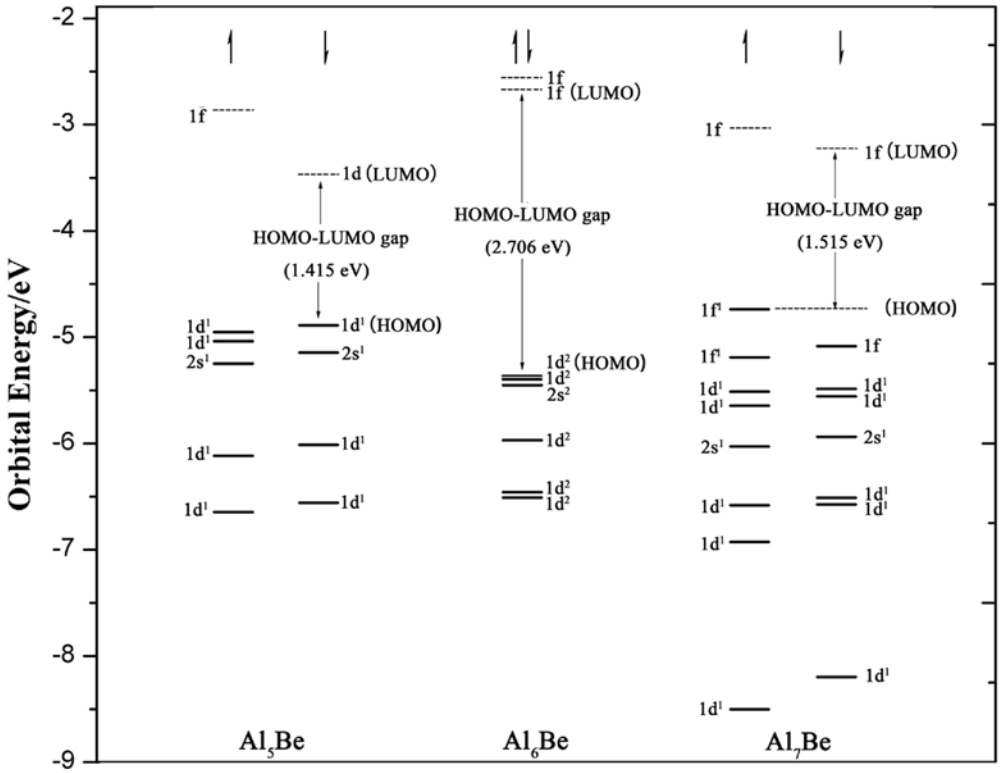

Figure S3. Orbital energies of valence 1d, 2s, and partial 1f orbitals of the Al_5Be, Al_6Be, and Al_7Be clusters. Occupied states are indicated by solid lines, and unoccupied ones by dotted lines.

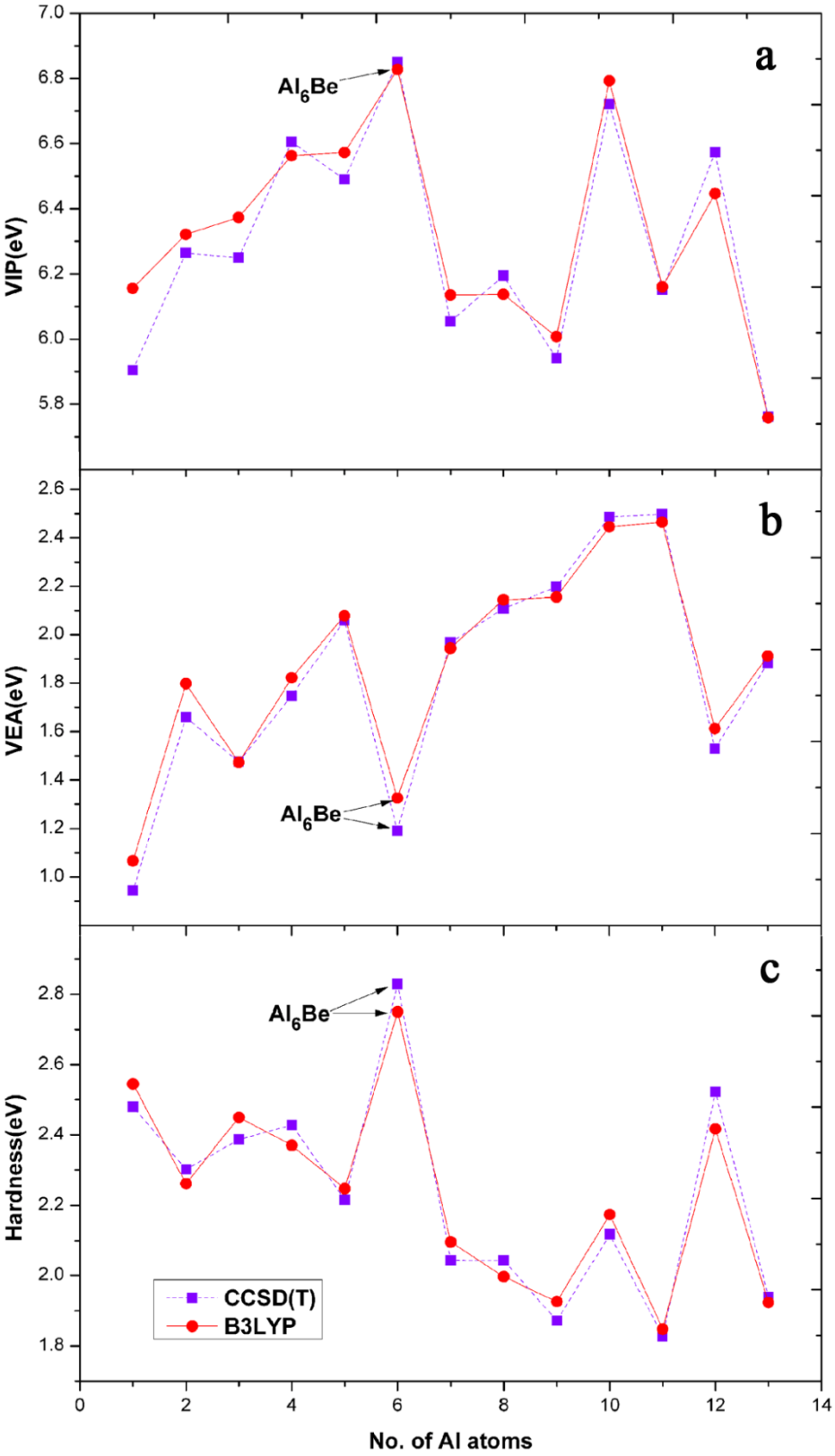

Figure S4. The (a) vertical ionization potentials (*VIP*s), (b) vertical electron affinities (*VEA*), (c) hardnesses (η, in eV) for the lowest-energy structures of Al_nBe clusters with $1 \leq n \leq 13$ at the CCSD(T)/aug-cc-pVDZ (dashed line) and B3LYP/aug-cc-pVDZ (solid line) levels, shown as a function of the number of Al atoms.

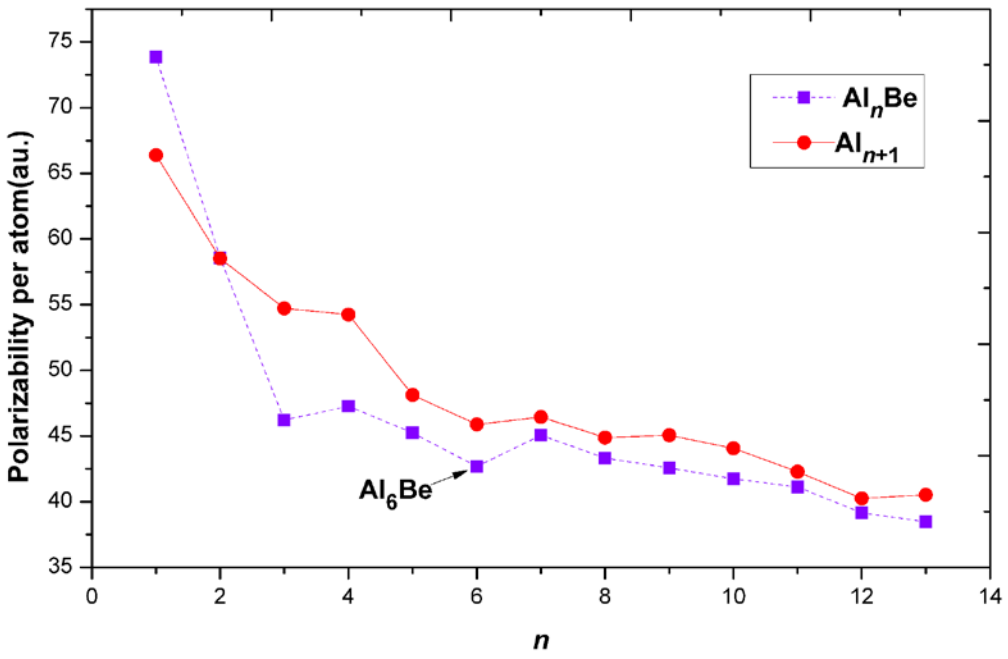

Figure S5. Polarizabilities per atom (in au.) for the lowest-energy structures of Al_nBe (dashed line) and Al_{n+1} clusters (solid line) at the B3LYP/aug-cc-pVDZ level, shown as a function of *n*.