Evolution of structure and properties of neutral and negatively charged transition metal-coronene complexes: A comprehensive analysis

Supplementary Information

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Table S1 The calculated vertical electron affinities (eV) for the coronene molecule at different levels, and compared with the experiment values.

Methods	PW91	B3PW91	B3LYP	BP86	TPSS	PBE	wB97XD	**Exp.**
LANL2DZ	0.46	0.33	0.26	0.53	0.34	0.43	0.04	
CEP-121G	0.56	0.20	0.34	0.62	0.46	0.56	0.18	
6-311+G	0.61	0.42	0.39	0.66	0.45	0.56	0.15	**0.54±0.1**[b]
6-31+G	0.58	0.39	0.36	0.62	0.42	0.54	0.21	
6-31+G*	0.63	0.44	0.40	0.67	0.45	0.59	0.17	

[b]Ref 42

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Fig. S1 Optimized structures of the low-lying neutral and anionic V_n(coronene)$_m$ complexes.

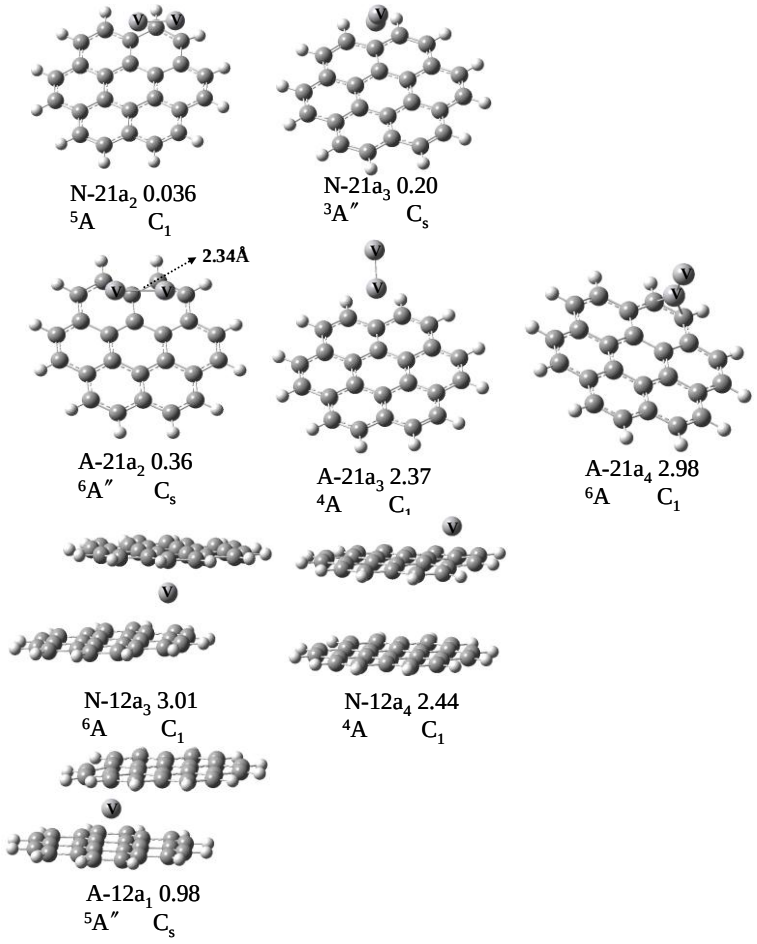

Fig. S2 Optimized structures of the low-lying neutral and anionic $Ti_n(coronene)_m$ complexes.

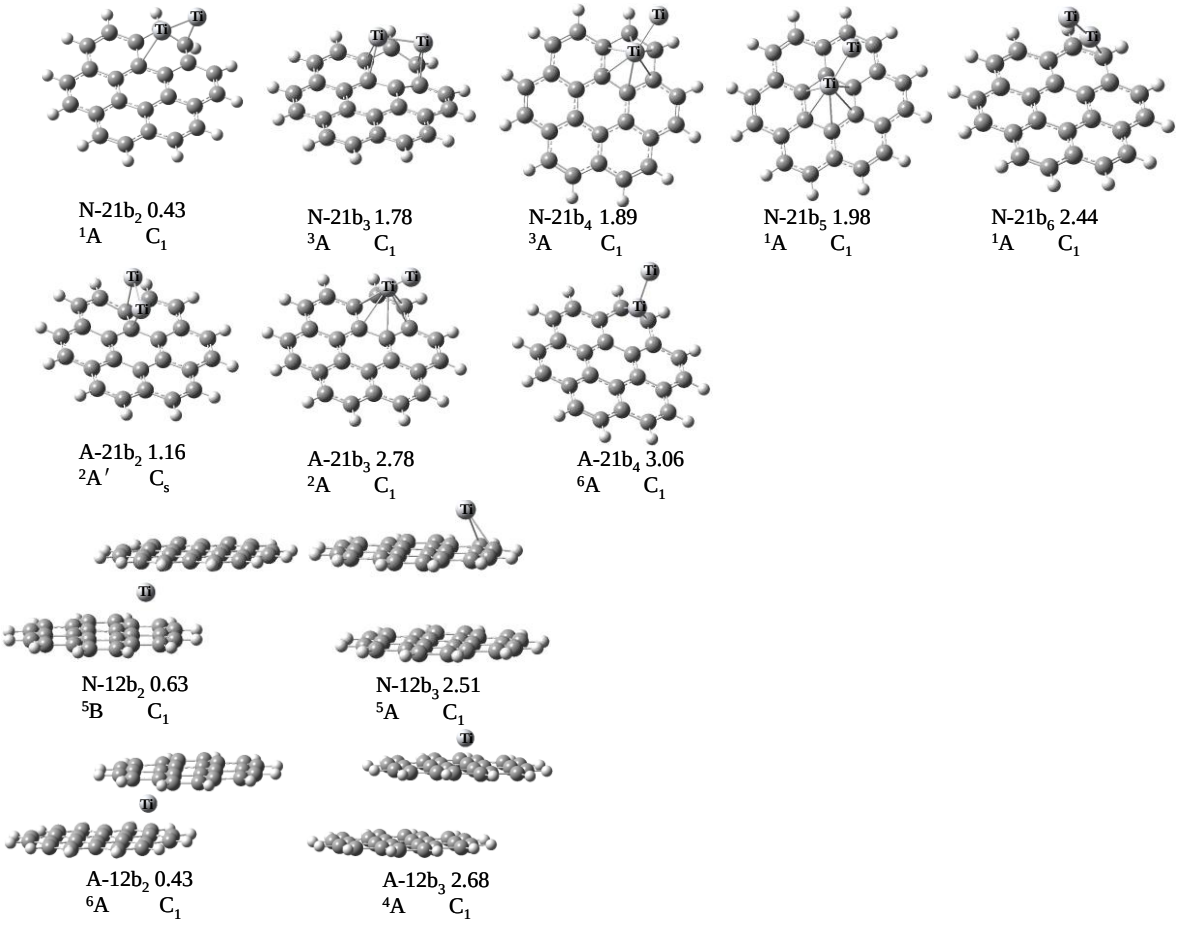

Fig. S3 Photoelectron spectra of $V(coronene)^-$ and $V_2(coronene)^-$ clusters.

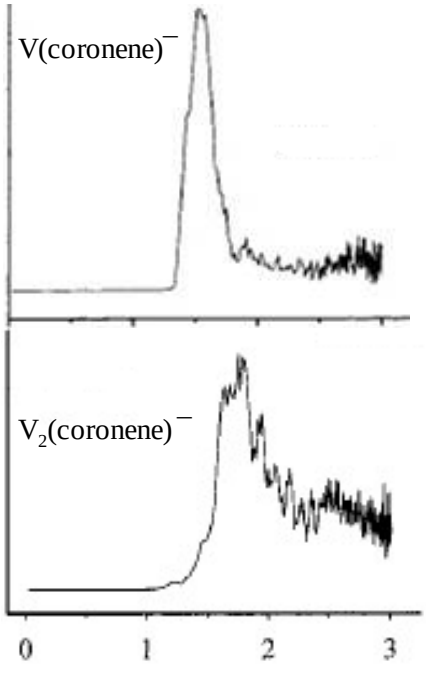

Fig. S4 The HOMO-1 and HOMO-2 of the ground state structures of $V_n(coronene)_m^{0/-}$. The first column corresponds to α molecular orbitals, while the second corresponds to β MOs.

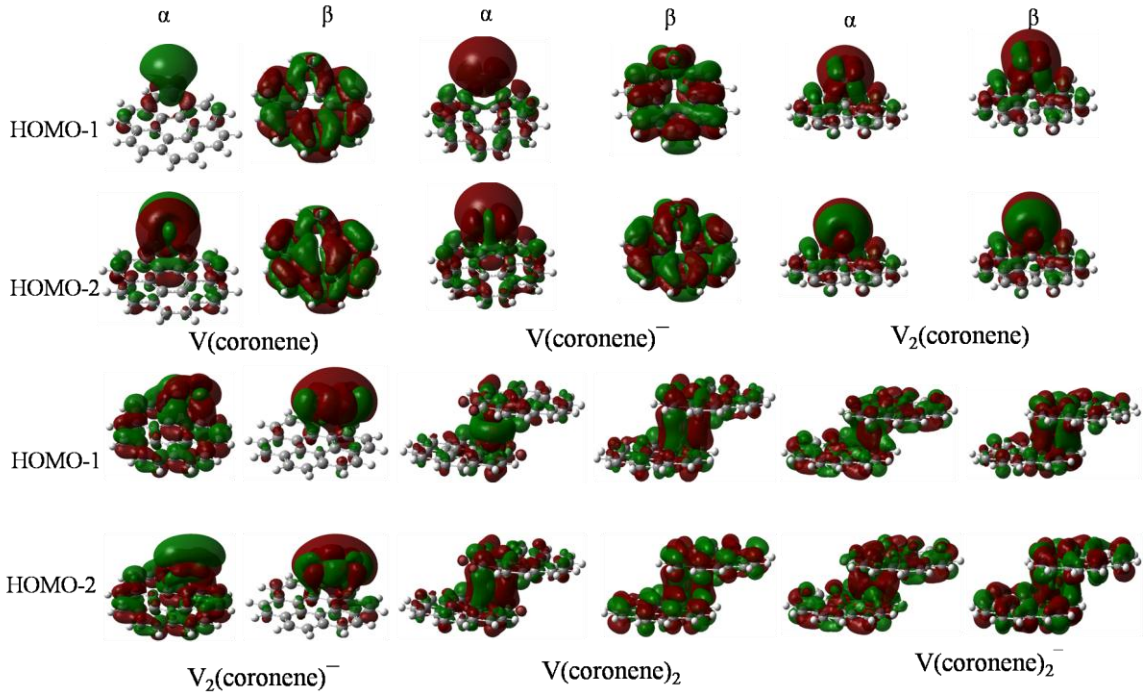

Fig. S5 The HOMO-1 and HOMO-2 of the ground state structures of $Ti_n(coronene)_m^{0/-}$. The first column corresponds to α molecular orbitals, while the second corresponds to β MOs.