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

Supplementary Information

Insights into the effects produced by doping of medium-sized boron clusters with Ruthenium

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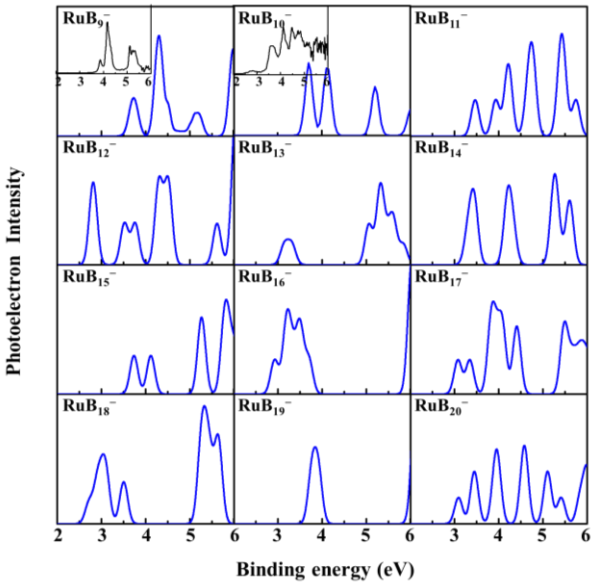

Figure S1. Our simulated photoelectron spectra of the lowest total energy states of RuB_n^- (n = 9-20) clusters with the experimental PES from Romanescu *et al*[1] for comparison.

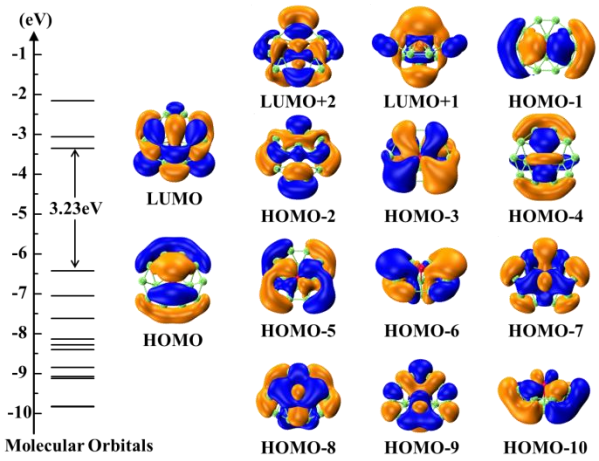

Figure S2. Molecular orbitals of the RuB_{14} cluster.

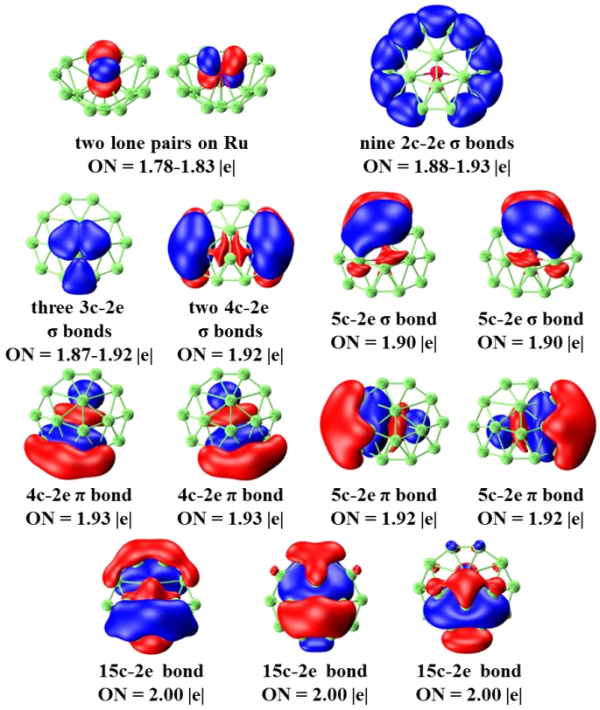

Figure S3. Chemical bonding patterns of the RuB_{14} cluster according to the results of the AdNDP analysis. "ON" stands for the occupation number.

Table S1. Compare the calculated vertical and adiabatic electron detachment energies with available experimental data.

Cluster	VDE(eV)		ADE(eV)	
	Theo.	Exp.	Theo.	Exp.
RuB_9^-	3.75	3.85[a]	3.65	3.83±0.02[a]
RuB_{10}^-	3.72	3.61[a]	3.51	3.35[a]
RuB_{11}^-	3.47		3.52	
RuB_{12}^-	3.52		2.73	
RuB_{13}^-	3.14		3.00	
RuB_{14}^-	3.31		2.90	
RuB_{15}^-	3.73		3.15	
RuB_{16}^-	2.92		2.71	
RuB_{17}^-	3.35		2.77	
RuB_{18}^-	3.02		2.72	
RuB_{19}^-	3.77		3.55	
RuB_{20}^-	3.09		2.96	

[a] Ref.1.

REFERENCE

1. Romanescu, C.; Galeev, T. R.; Li, W. L.; Boldyrev, A. I.; Wang, L. S. Aromatic Metal-Centered Monocyclic Boron Rings: Co©B_8^- and Ru©B_9^-. *Angew. Chem. Int. Ed.* **2011**, *50*, 9334−9337.

Table S2. The calculated relative energy (ΔE) values for $RuB_{12}^{0/-}$ and $RuB_{14}^{0/-}$ clusters at the CCSD(T)/Stuttgart/Ru/6-311+G(d)/B level of theory.

Isomers		ΔE (eV)	Isomers		ΔE (eV)
RuB_{12}	12n-1	0.00	RuB_{12}^-	12a-1	0.00
	12n-2	0.34		12a-2	0.97
	12n-3	1.17		12a-3	1.20
RuB_{14}	14n-1	0.00	RuB_{14}^-	14a-1	0.00
	14n-2	0.25		14a-2	0.76
	14n-3	2.05		14a-3	2.19