

Electronic Supporting Information

Electronic Structure and Chemical Bonding in the Double Ring Tubular Boron Clusters

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The supporting information file includes:

- Table S1 defining the parameters of a double ring cylinder.
- Figure S1: Geometries of the B_{2n} DR's.
- Figure S2: determination of the *k* parameter.
- Figures S3, S4 and S5: Total and partial densities of state maps.

Table S1. The hollow cylinder parameters of π -MOs set of DR B₂₀ , B₂₄ , B₂₈ . The radius R and the length L of these structures are determined from their coordinates. The active radius and the length of these hollow cylinder are calculated by $r_{\pi} = R \cdot \varepsilon_{\pi}$ and $L_{\pi} = R \cdot L_{\pi}^f$, respectively.

B _{2n}		B ₂₀	B ₂₄	B ₂₈
R (Å)		2.601	3.122	3.602
L (Å)		1.510	1.467	1.524
π -MOs	ε_{π}	0.863	0.762	0.696
	L_{π}^f	1.415	1.151	1.068
	r_{π} (Å)	2.245	2.379	2.507
	L_{π} (Å)	3.680	3.593	3.847

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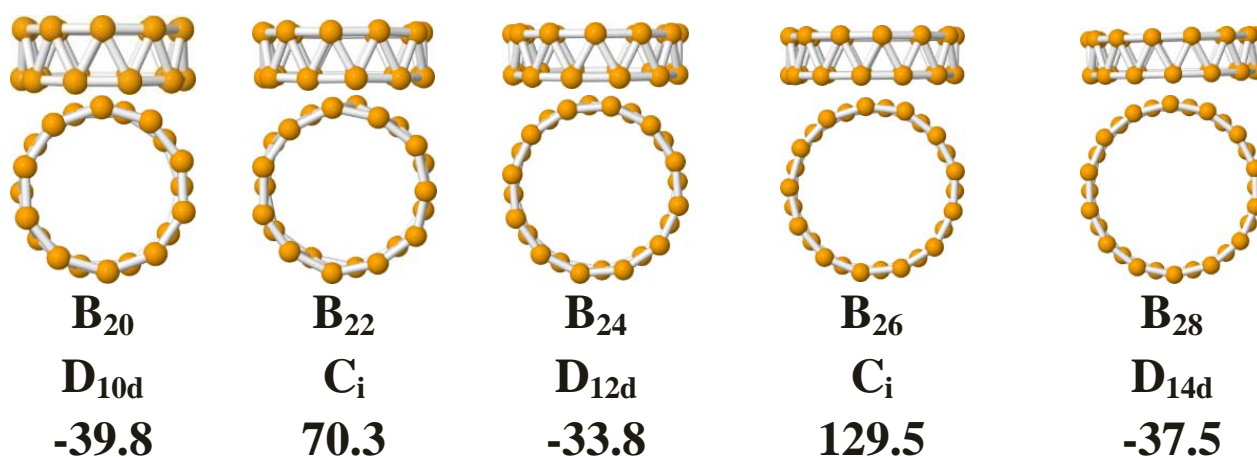


Figure S1. The geometries of B_{2n} clusters with n = 10,11,12,13,14 DR structures, and their NICS(0.0) values. Geometrical optimizations were performed using TPSSh/6-311+g(d) computations, the NICS(0) values were given by GIAO method at the same level of theory.

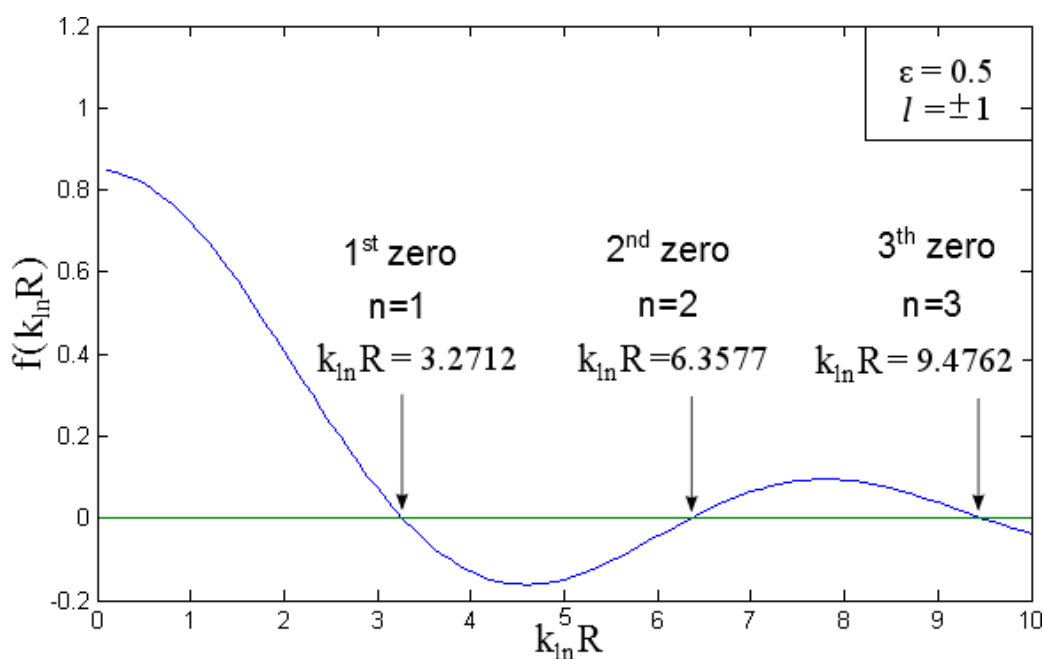


Figure S2. Method of determination for $k_{ln}R$. Graph shows the first three $k_{ln}R$ values of Eq.(4) when $\varepsilon = 0.5$ and $l = \pm 1$.

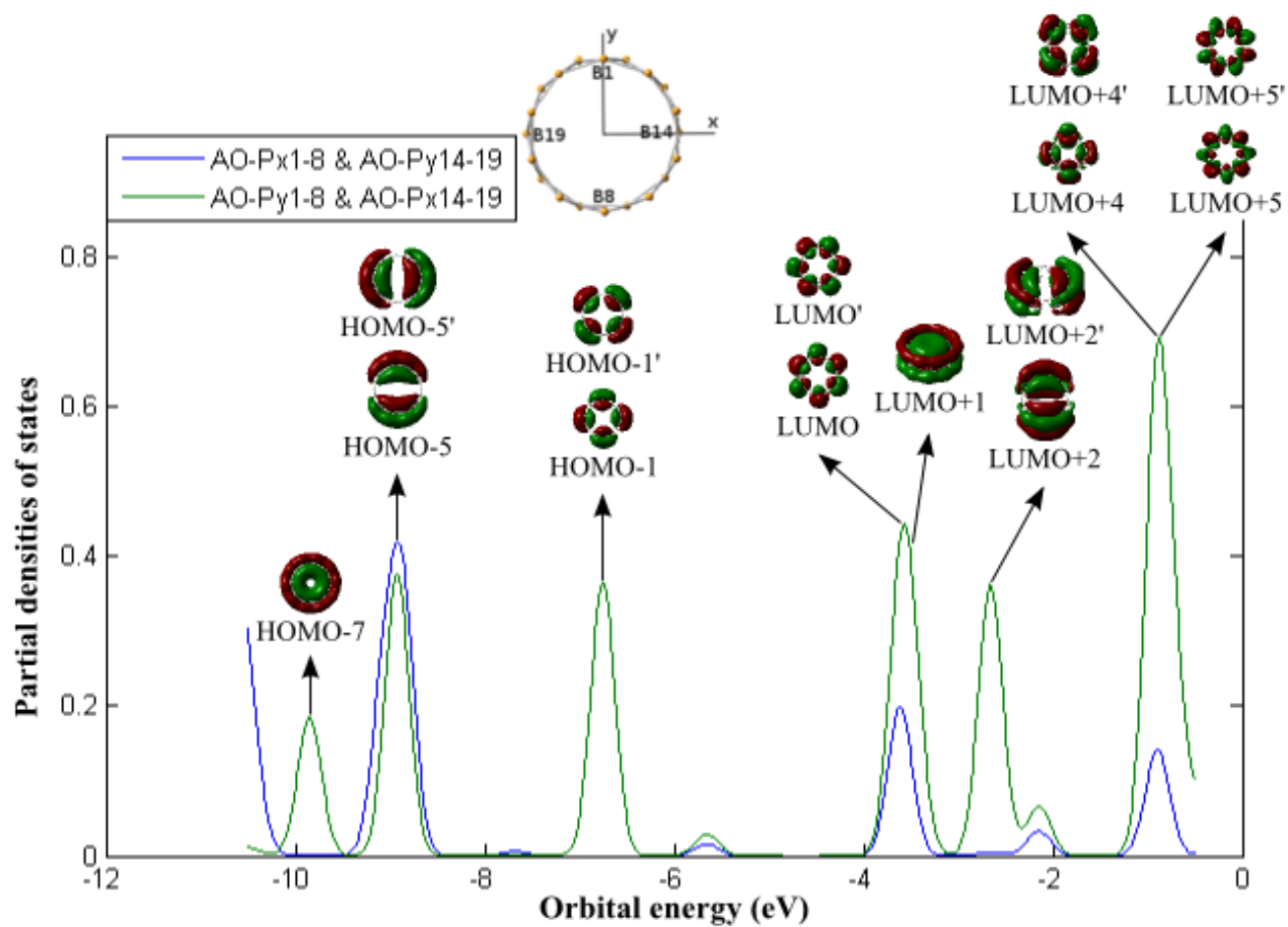


Figure S3. Partial (pDOS) densities of state of B_{20} DR.

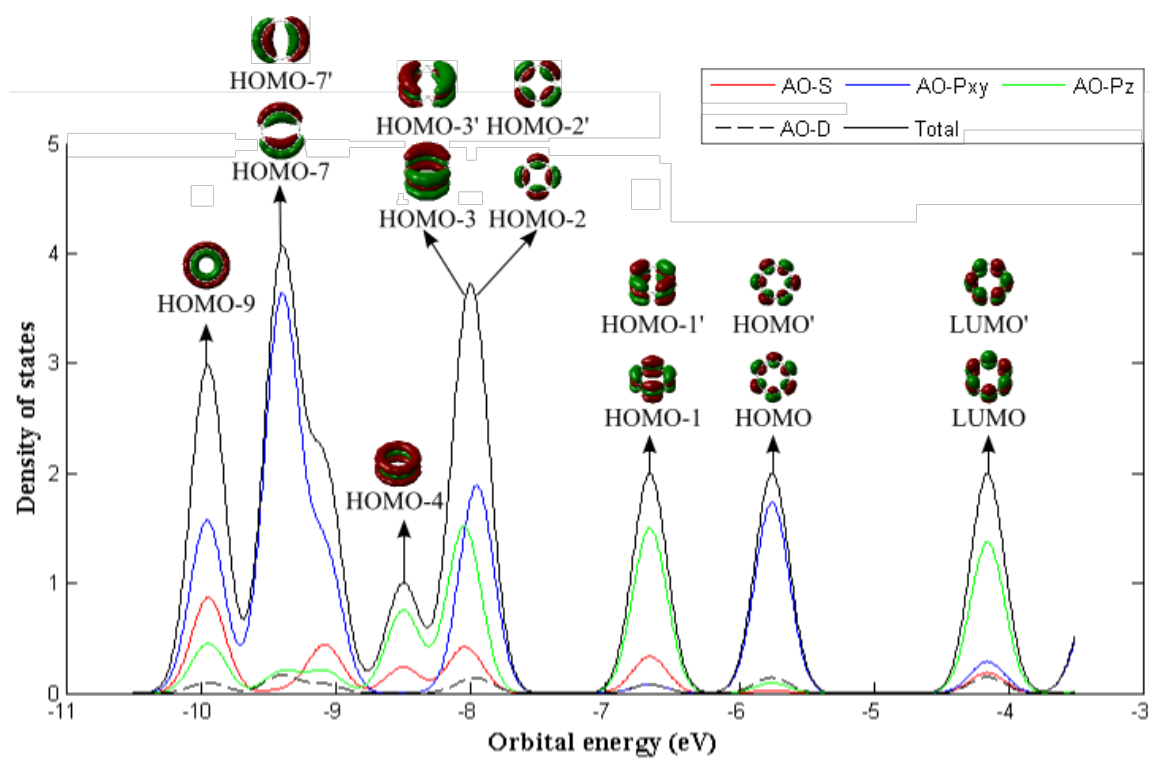


Figure S4. Total (DOS) and partial (pDOS) densities of state of B₂₄ DR.

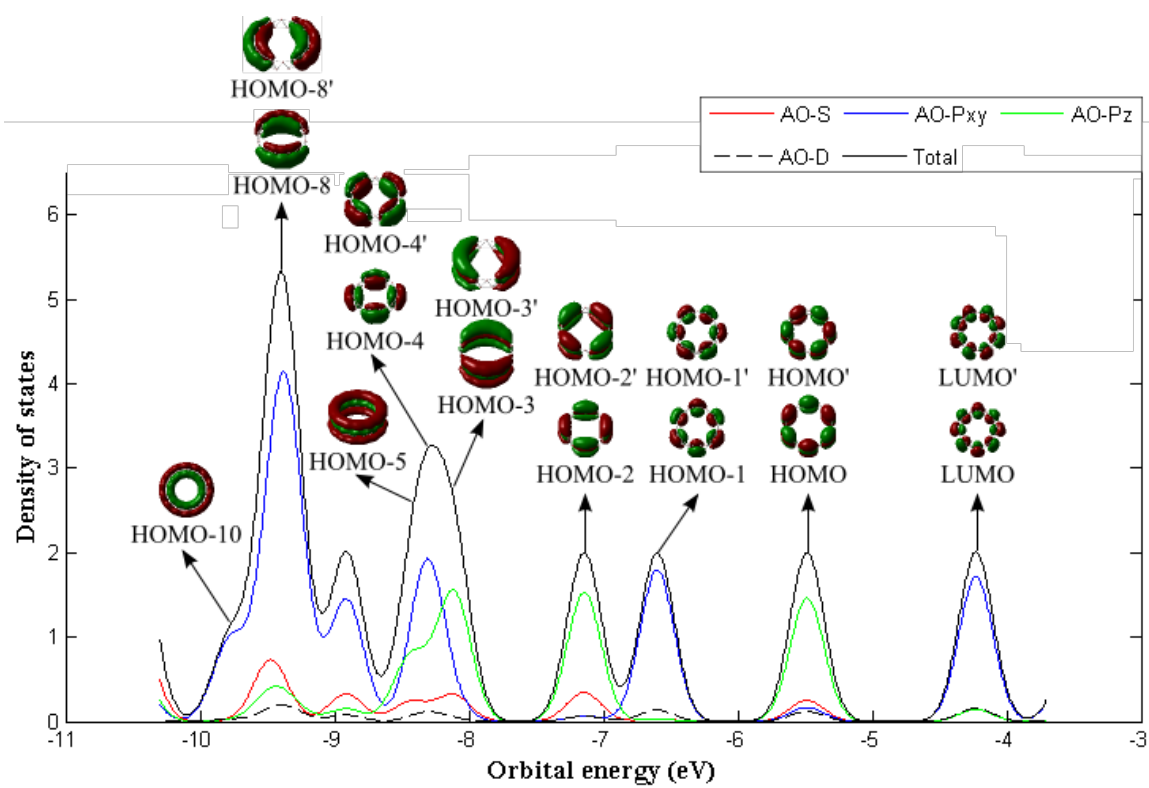


Figure S5. Total (DOS) and partial (pDOS) densities of state of B₂₈ DR.