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SUPPLEMENTARY INFORMATION

B_{11}^-: A Moving Subnanoscale Tank Tread

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SUPPLEMENTARY INFORMATION – PART I.

Table S1. Cartesian coordinates for the global-minimum structures of B_{11}^- C_{2v} ($^1A_1$), B_{11} C_{2v} ($^2B_2$), and their corresponding C_{2v} transition states at the PBE0/6-311+G* level.

Figure S1. Optimized structures of (a) C_{2v} ($^1A_1$) global minimum (GM) and (b) C_{2v} ($^1A_1$) transition state (TS) of B_{11}^- at PBE0/6-311+G* level. The bond distances are indicated in Å.

Figure S2. Optimized structures of the C_{2v} ($^2B_2$) global minimum (GM) and the C_{2v} transition state (TS) of the B_{11} neutral cluster at the PBE0/6-311+G* level. The bond distances are indicated in Å.

Figure S3. The total electron localization function (ELF) of the B_{11}^- C_{2v} ($^1A_1$) global minimum.

Figure S4. Chemical bonding in the C_{2v} transition state of B_{11}^-. (a) The electron localization functions (ELFs), including the total ELF. (b) Bonding elements as revealed using the adaptive natural density partitioning (AdNDP) analysis.

Figure S5. Schematic representation of the structural evolution during the peripheral rotation of the B_{11} cluster.

SUPPLEMENTARY INFORMATION – PART II.

A short movie extracted from the BOMD simulation for B_{11}^-. Each frame of the snapshot is reoriented horizontally. The simulation is performed at 300 K for over 20 ps and the movie roughly covers a 4 ps time span.

Fig. S1. Optimized structures of (a) C_{2v} ($^1A_1$) global minimum (GM) and (b) C_{2v} ($^1A_1$) transition state (TS) of B_{11}^- at PBE0/6-311+G* level. The bond distances are indicated in Å.

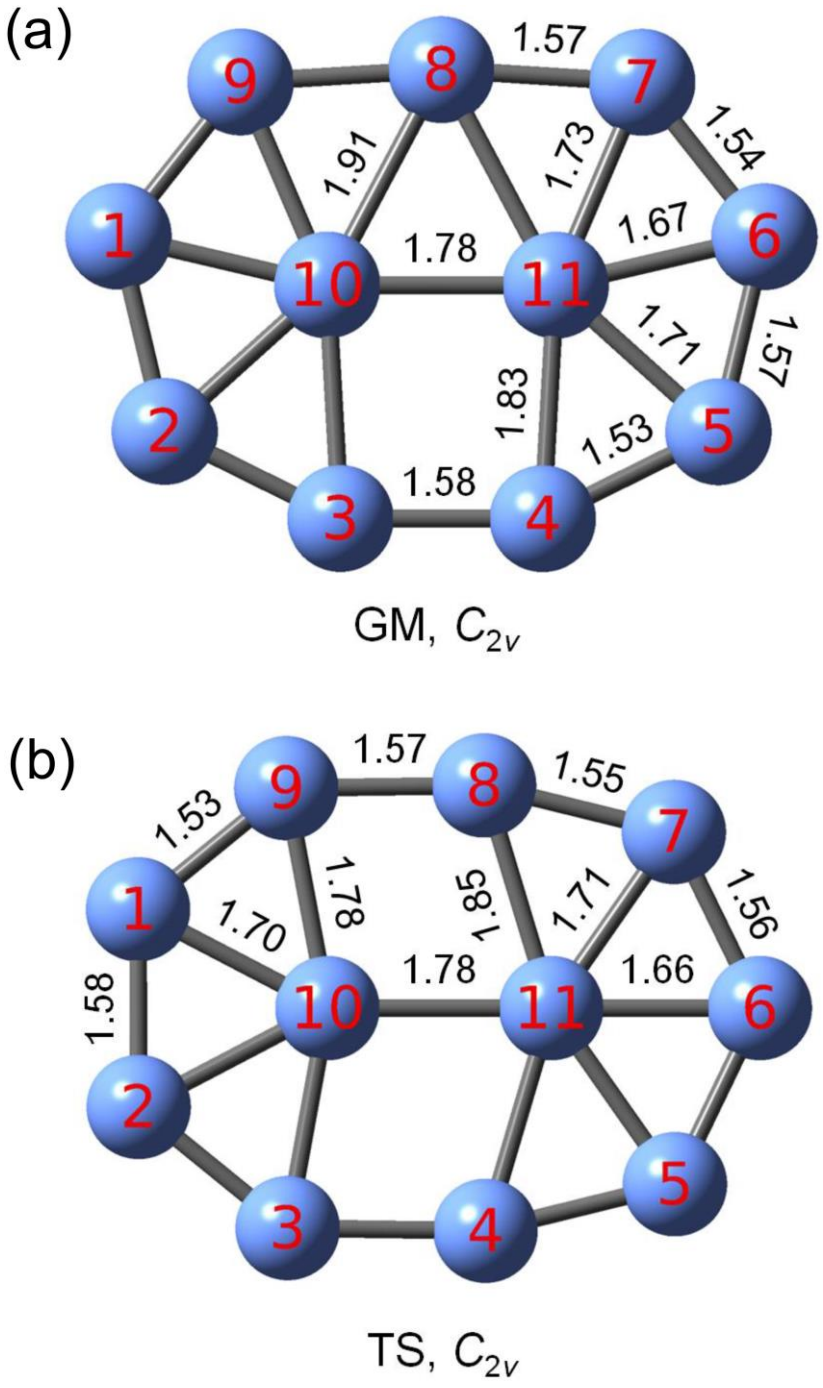

Fig. S2. Optimized structures of the C_{2v} ($^2B_2$) global minimum (GM) and the C_{2v} ($^2B_2$) transition state (TS) of the B_{11} neutral cluster at the PBE0/6-311+G* level. The bond distances are indicated in Å.

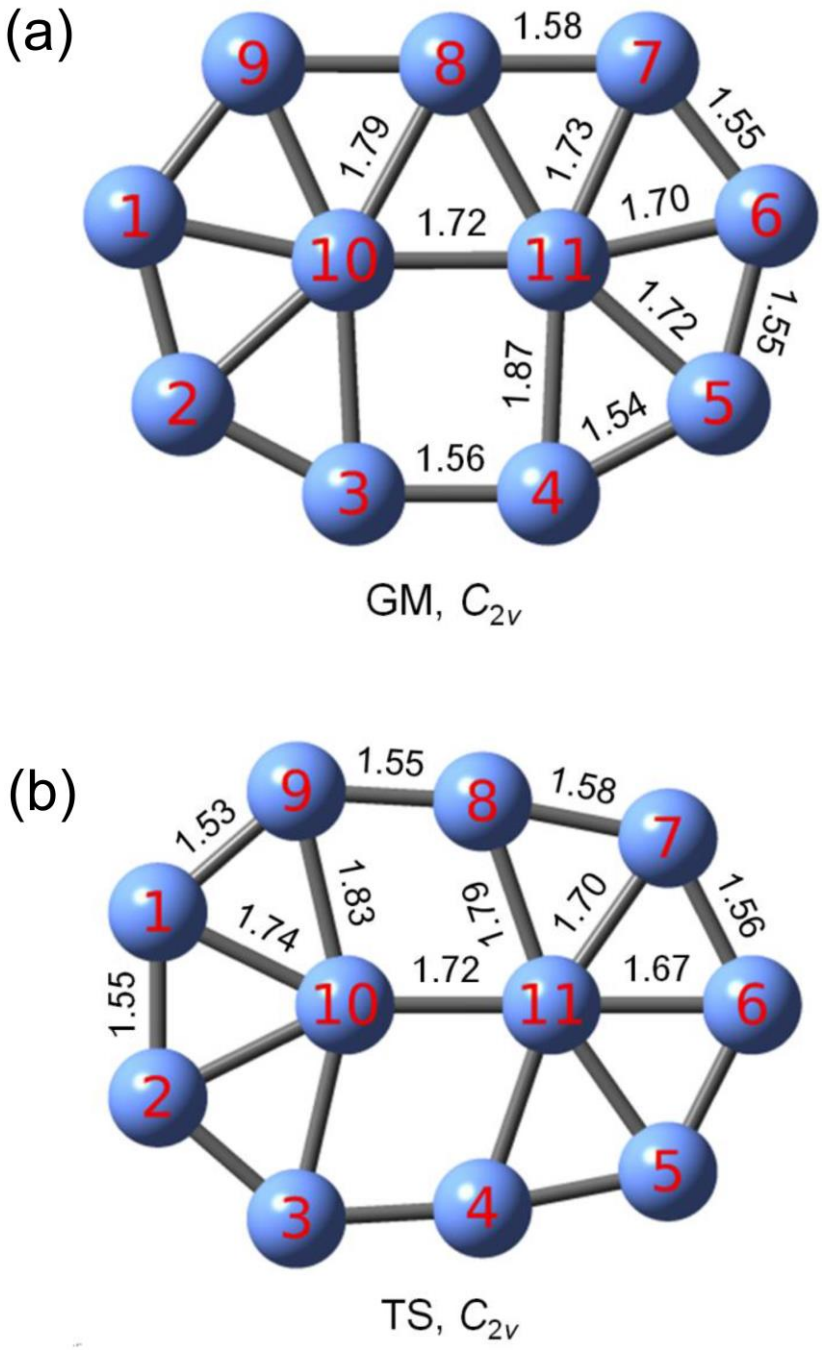

Fig. S3. The total electron localization function (ELF) of the B_{11}^- C_{2v} ($^1A_1$) global minimum.

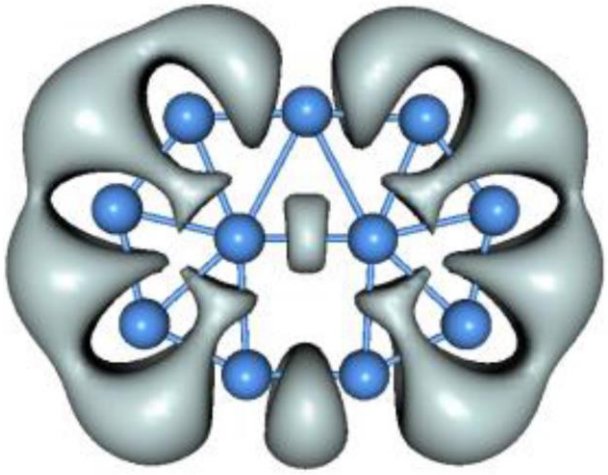

Fig. S4. Chemical bonding in the C_{2v} transition state of B_{11}^-. (a) The electron localization functions (ELFs). (b) Bonding elements as revealed using the adaptive natural density partitioning (AdNDP) analysis. Note that two diagonal bonds at the right side are 4c-2e σ bonds.

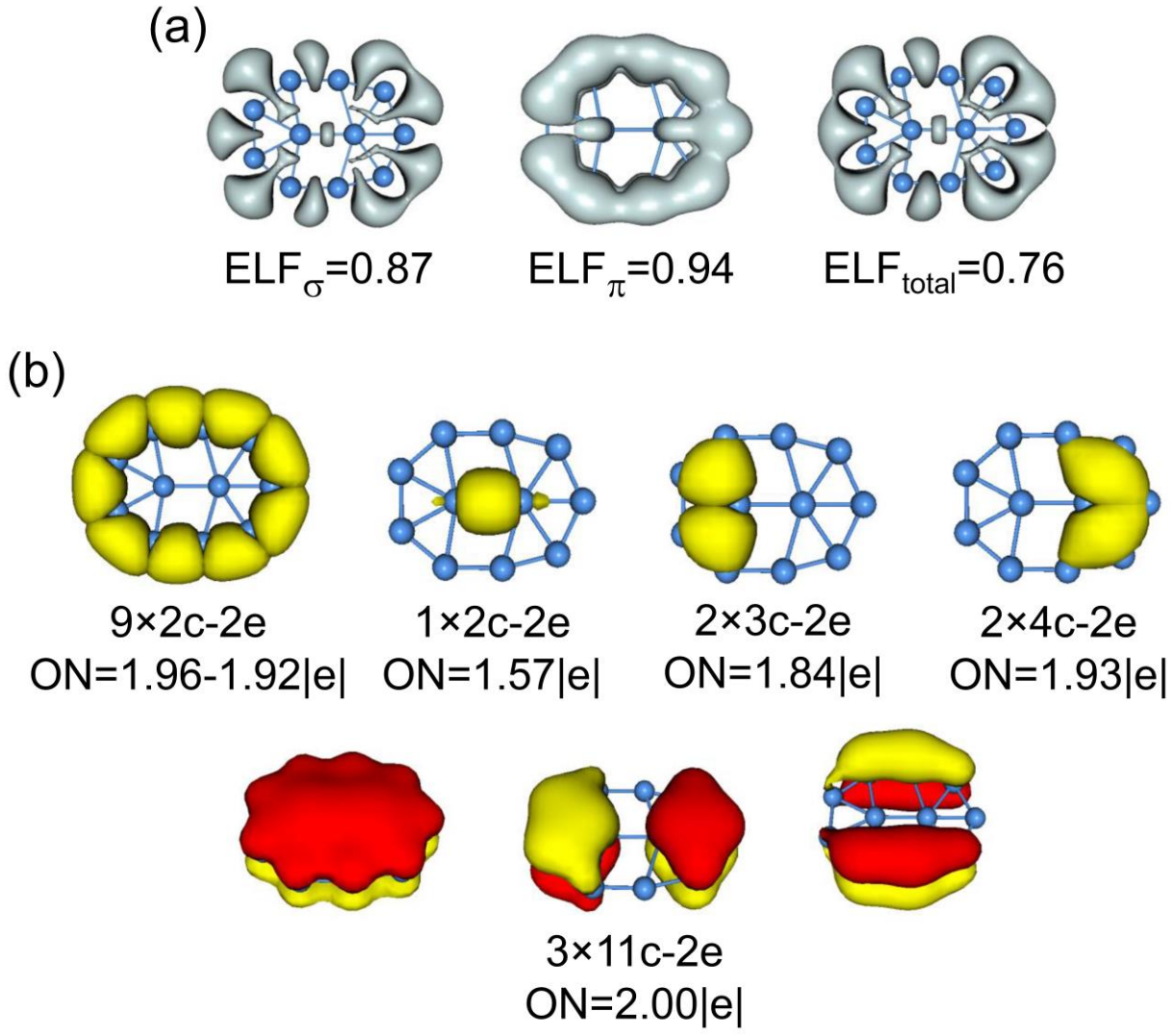

Fig. S5. Schematic representation of the structural evolution during the peripheral rotation of the B_{11} cluster.

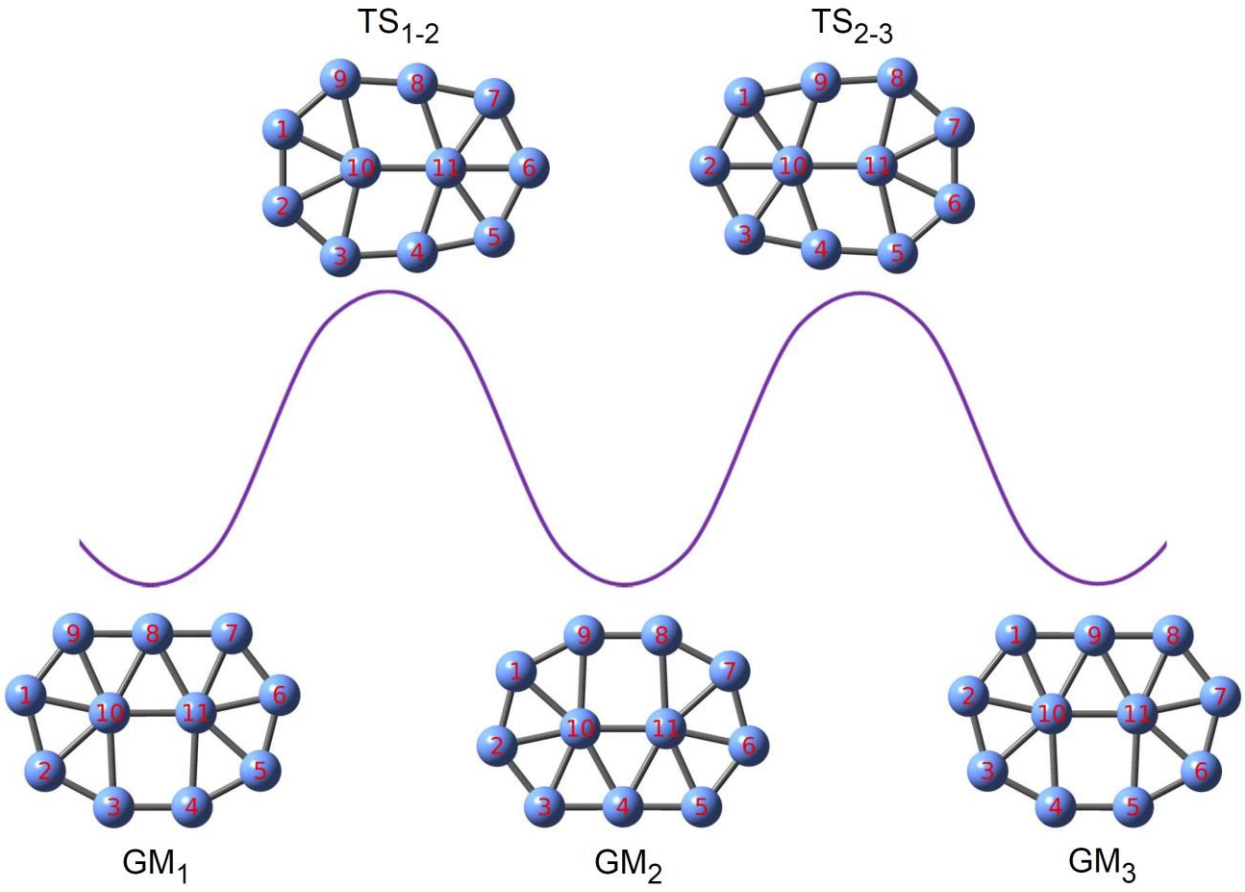

Table S1. Cartesian coordinates for the global-minimum (GM) structures of B_{11}^- C_{2v} ($^1A_1$), B_{11} C_{2v} ($^2B_2$), and their corresponding C_{2v} transition states (TS) at the PBE0/6-311+G* level.

(a) GM of B_{11}^- C_{2v} ($^1A_1$)

B	0.00000000	2.51850300	0.41101700
B	0.00000000	2.15908000	-1.11950100
B	0.00000000	0.78880700	-1.80161800
B	0.00000000	-0.78880700	-1.80161800
B	0.00000000	-2.15908000	-1.11950100
B	0.00000000	-2.51850300	0.41101700
B	0.00000000	-1.56602500	1.62109100
B	0.00000000	0.00000000	1.71913300
B	0.00000000	1.56602500	1.62109100
B	0.00000000	0.89122700	0.02944500
B	0.00000000	-0.89122700	0.02944500

(b) TS of B_{11}^- C_{2v}

B	0.00000000	0.78763400	-2.37444500
B	0.00000000	-0.78763400	-2.37444500
B	0.00000000	-1.75319900	-1.19307500
B	0.00000000	-1.77484700	0.37985000
B	0.00000000	-1.40357100	1.88642400
B	0.00000000	0.00000000	2.56556000
B	0.00000000	1.40357100	1.88642400
B	0.00000000	1.77484700	0.37985000
B	0.00000000	1.75319900	-1.19307500
B	0.00000000	0.00000000	-0.87073500
B	0.00000000	0.00000000	0.90766800

(c) GM of B_{11} C_{2v} ($^2B_2$)

B	0.00000000	2.52678400	0.40746800
B	0.00000000	2.14422800	-1.09562700
B	0.00000000	0.77774500	-1.81539800
B	0.00000000	-0.77774500	-1.81539800
B	0.00000000	-2.14422800	-1.09562700
B	0.00000000	-2.52678400	0.40746800
B	0.00000000	-1.57646300	1.63342000
B	0.00000000	0.00000000	1.62873900
B	0.00000000	1.57646300	1.63342000
B	0.00000000	0.86164900	0.05576700
B	0.00000000	-0.86164900	0.05576700

(d) TS of B_{11} C_{2v}

B	0.00000000	0.77309500	-2.36698300
B	0.00000000	-0.77309500	-2.36698300
B	0.00000000	-1.78199600	-1.21072900
B	0.00000000	-1.69621200	0.34016900
B	0.00000000	-1.39098200	1.88717500
B	0.00000000	0.00000000	2.58981600
B	0.00000000	1.39098200	1.88717500
B	0.00000000	1.69621200	0.34016900
B	0.00000000	1.78199600	-1.21072900
B	0.00000000	0.00000000	-0.80483200
B	0.00000000	0.00000000	0.91575000