

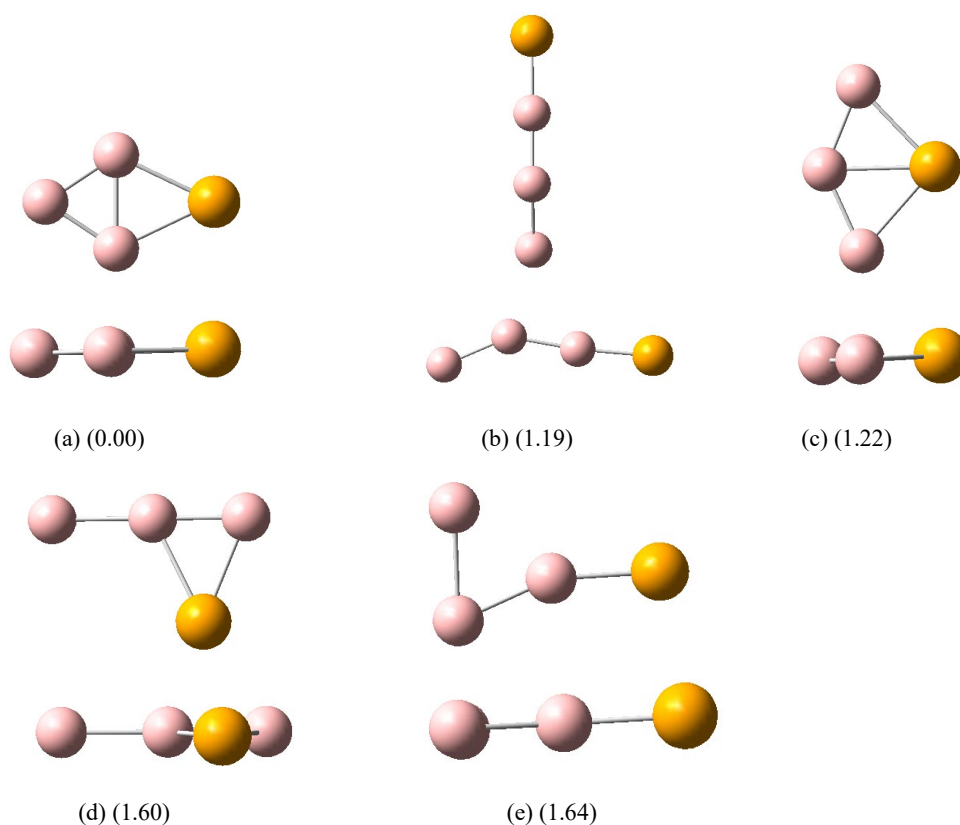
# Structural Evolution and Electronic Properties of Selenium-Doped Boron Clusters $\text{SeB}_n^{0/-}$ ( $n = 3-16$ )

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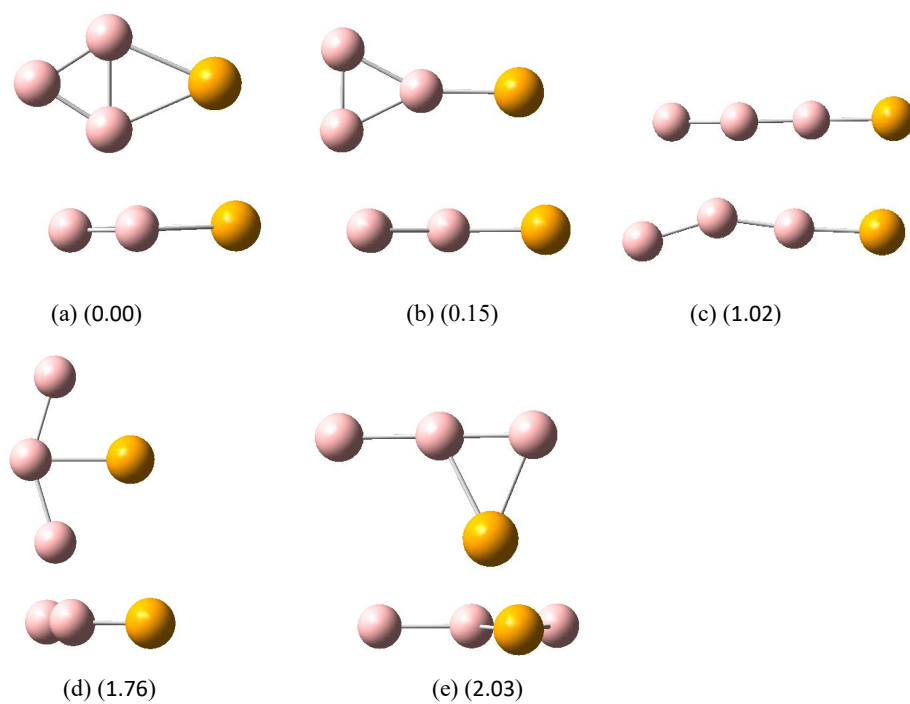
<sup>1</sup> School of Physics and Electronic Science, Guizhou Education University,  
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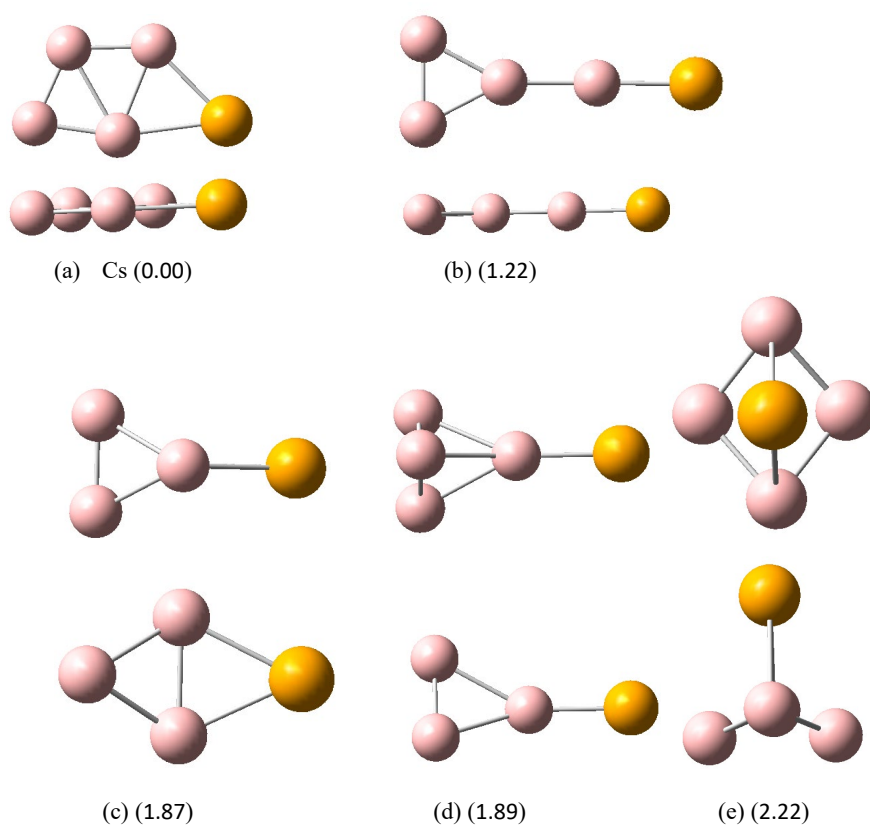
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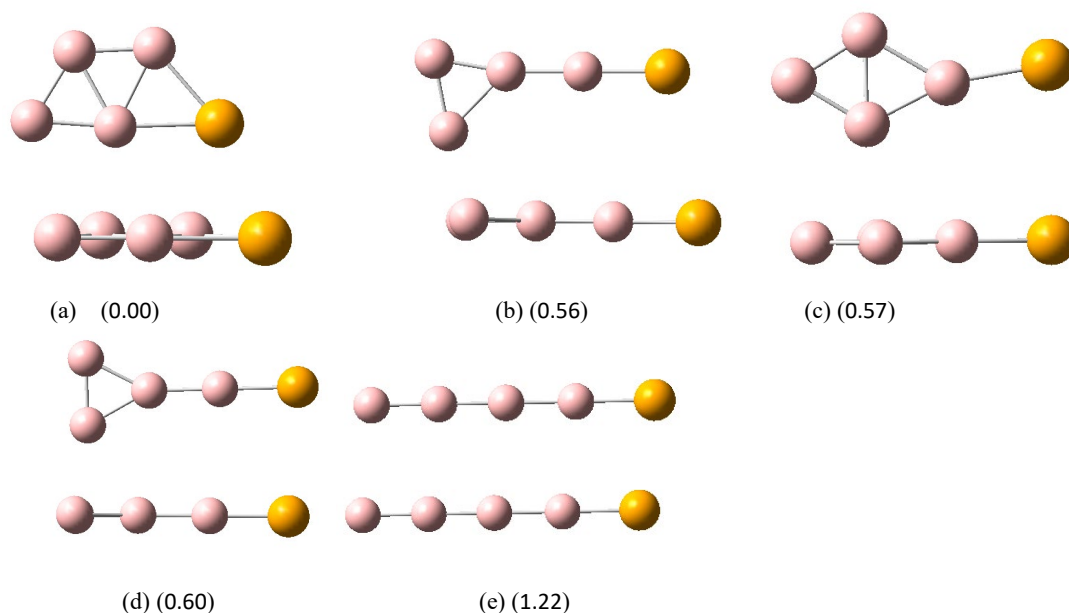
**Figure S1.** Low-lying isomers of doped boron clusters  $\text{SeB}_3$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_3$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



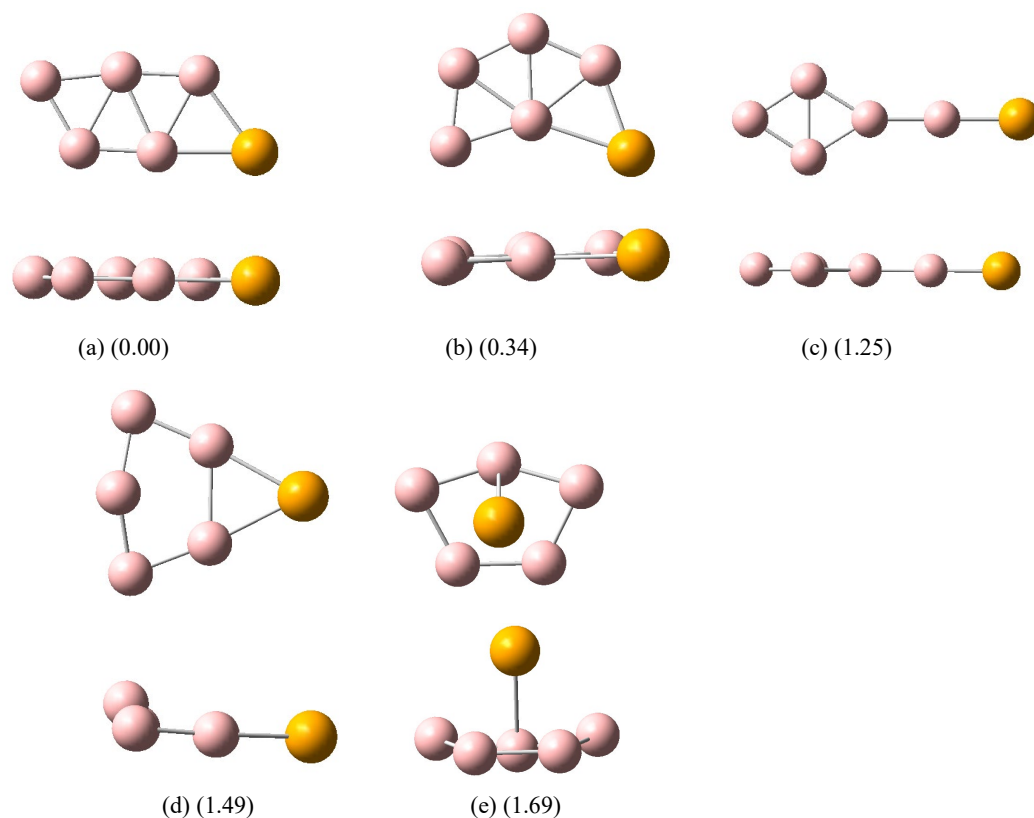
**Figure S2.** Low-lying isomers of doped boron clusters  $\text{SeB}_3^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_3^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



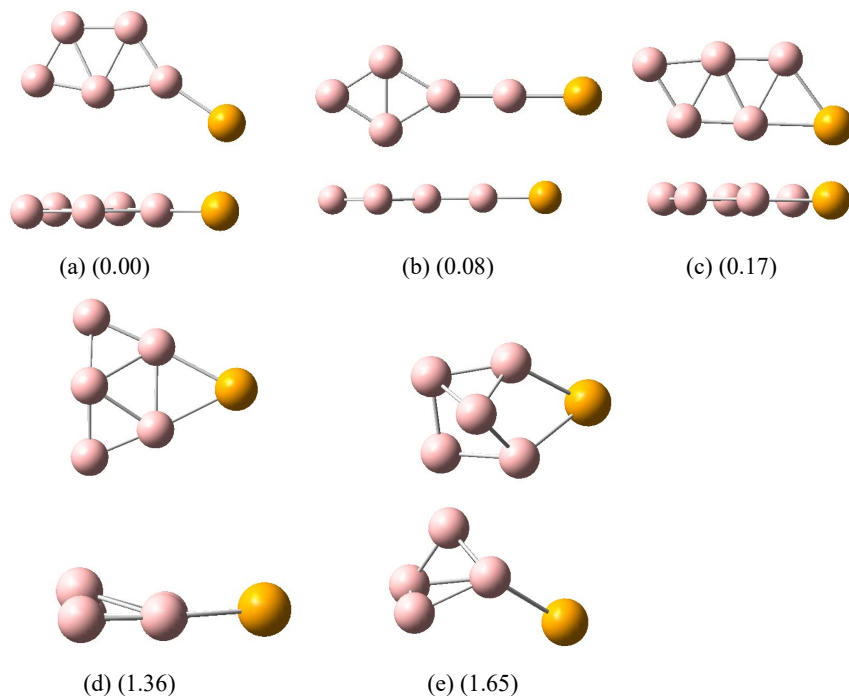
**Figure S3.** Low-lying isomers of doped boron clusters  $\text{SeB}_4$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_4$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



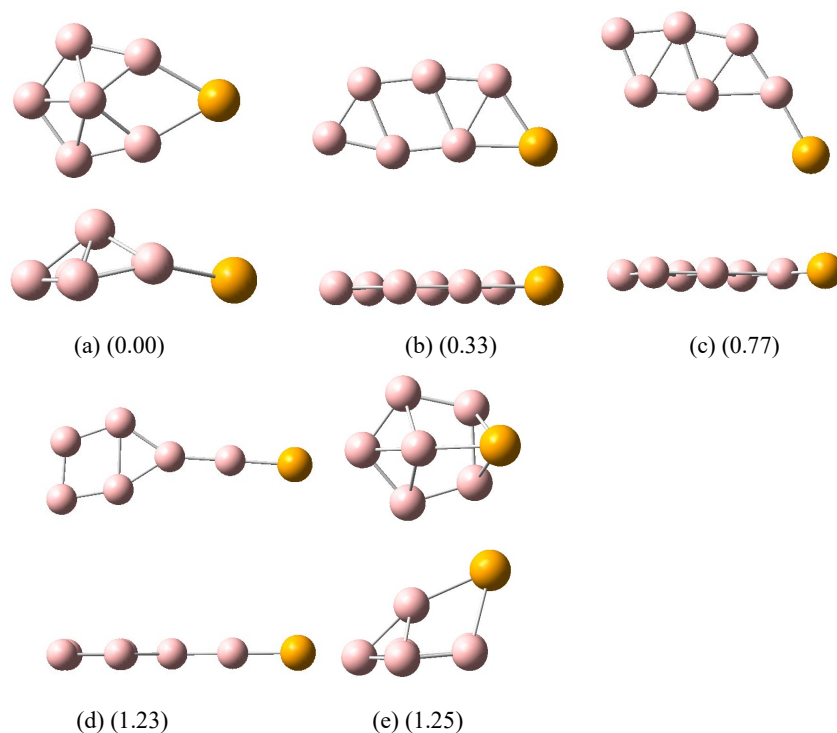
**Figure S4.** Low-lying isomers of doped boron clusters  $\text{SeB}_4^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_4^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



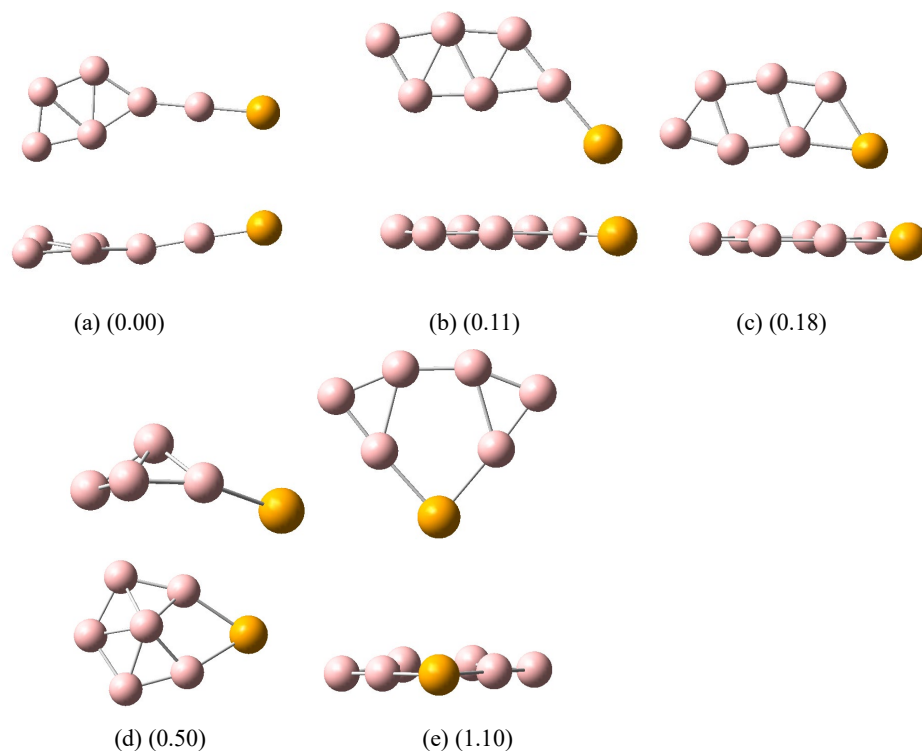
**Figure S5.** Low-lying isomers of doped boron clusters  $\text{SeB}_5$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_5$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



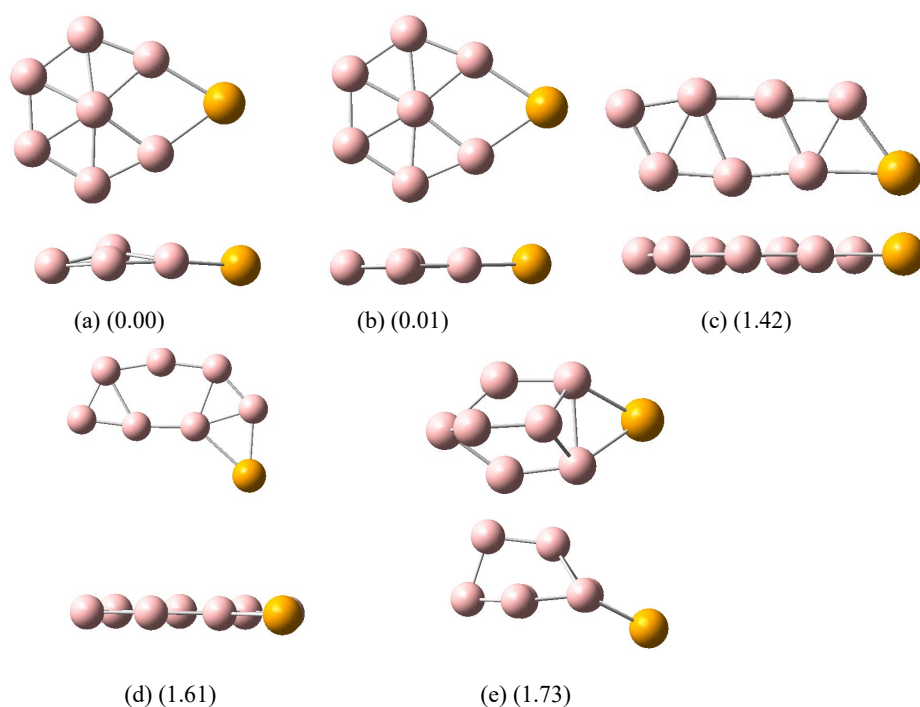
**Figure S6.** Low-lying isomers of doped boron clusters  $\text{SeB}_5^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_5^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



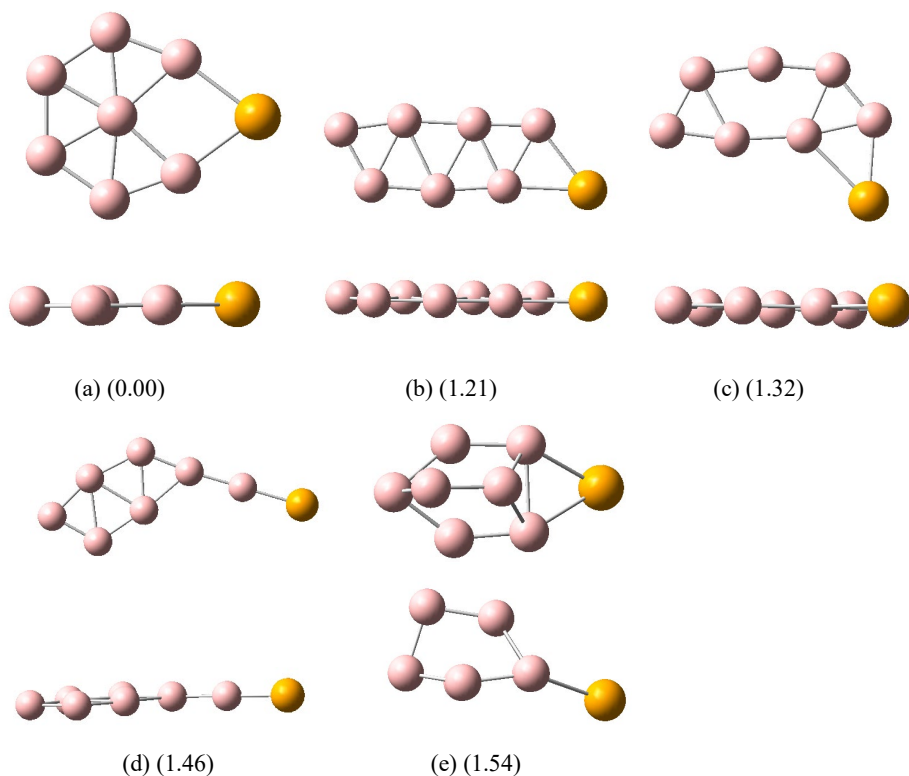
**Figure S7.** Low-lying isomers of doped boron clusters  $\text{SeB}_6$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_6$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



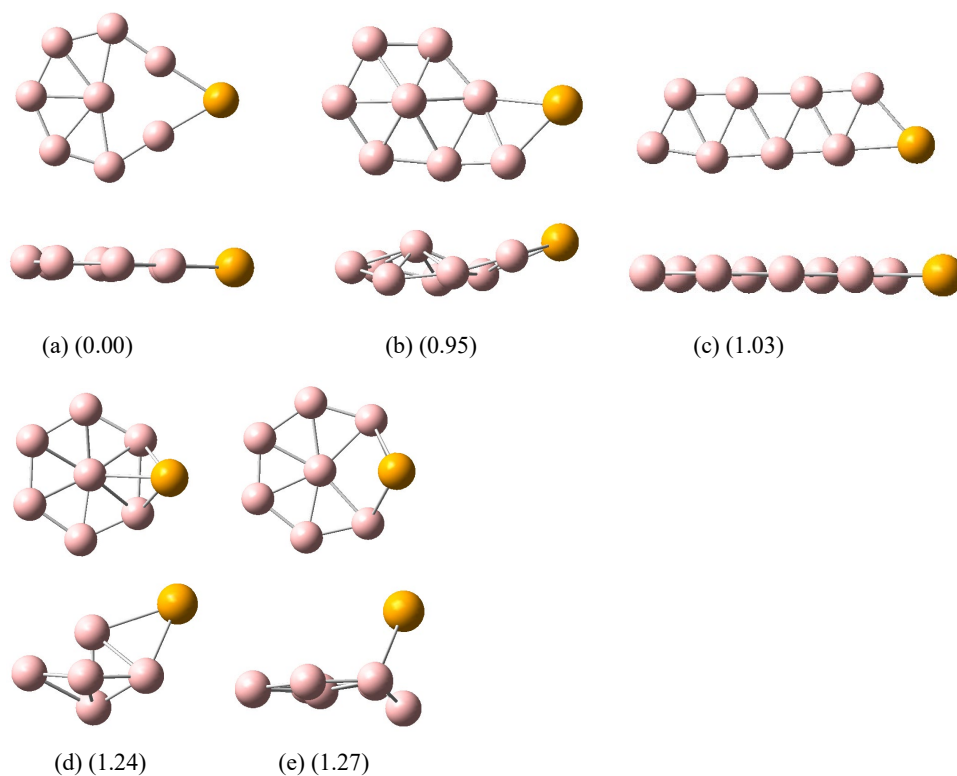
**Figure S8.** Low-lying isomers of doped boron clusters  $\text{SeB}_6^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_6^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



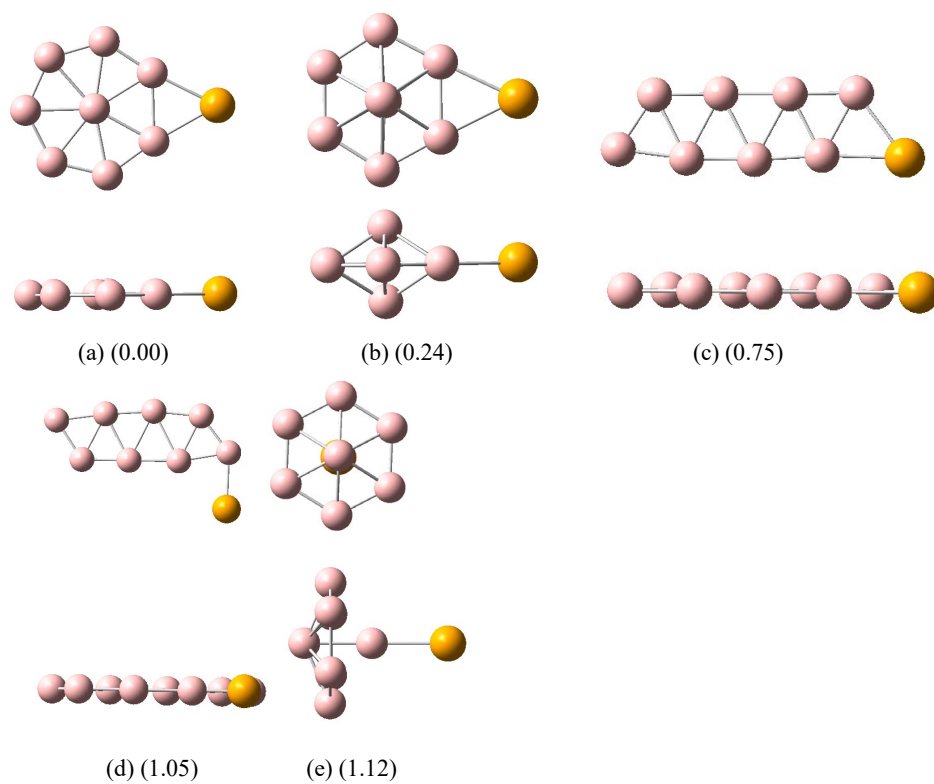
**Figure S9.** Low-lying isomers of doped boron clusters  $\text{SeB}_7$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_7$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



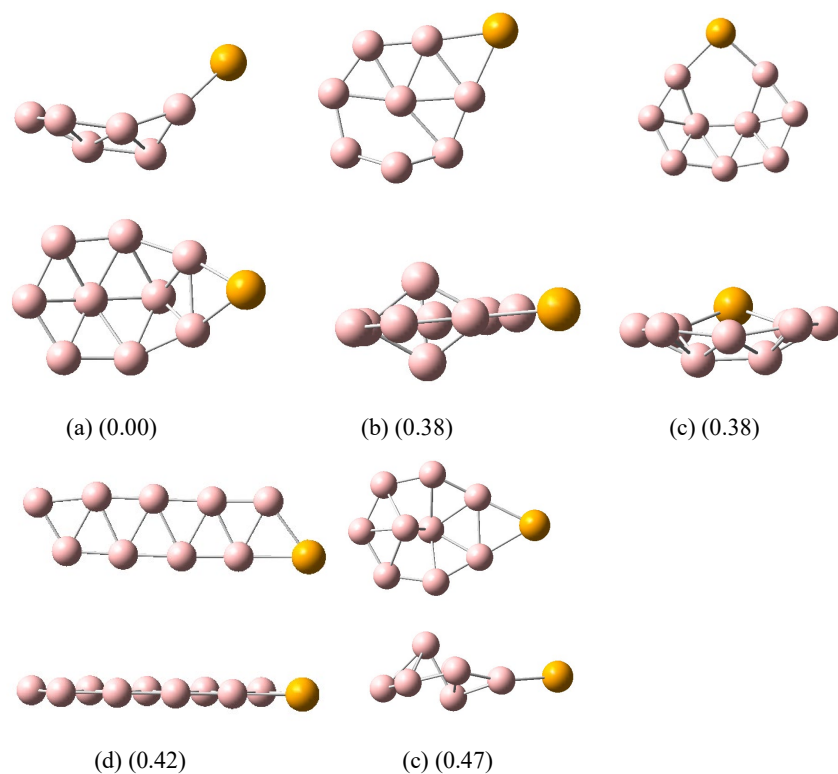
**Figure S10.** Low-lying isomers of doped boron clusters  $\text{SeB}_7^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_7^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



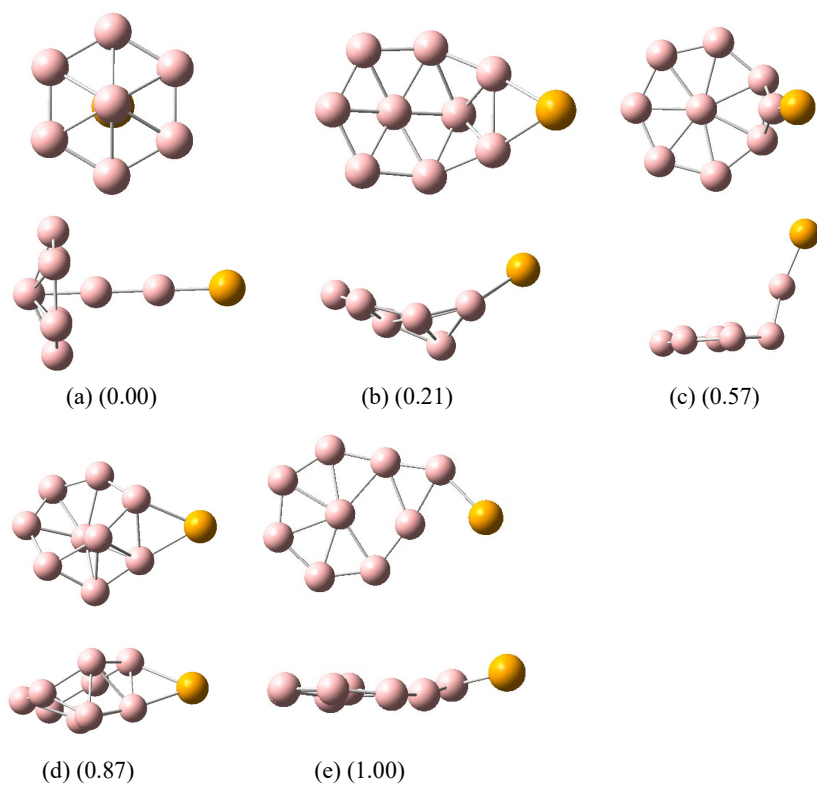
**Figure S11.** Low-lying isomers of doped boron clusters  $\text{SeB}_8$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_8$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



**Figure S12.** Low-lying isomers of doped boron clusters  $\text{SeB}_8^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_8^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

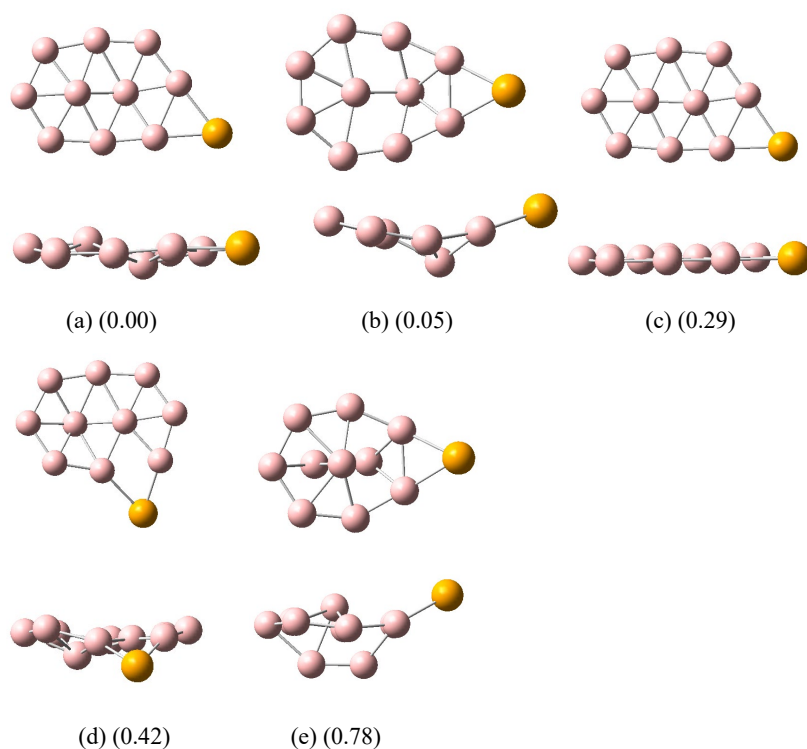


**Figure S13.** Low-lying isomers of doped boron clusters  $\text{SeB}_9$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_9$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

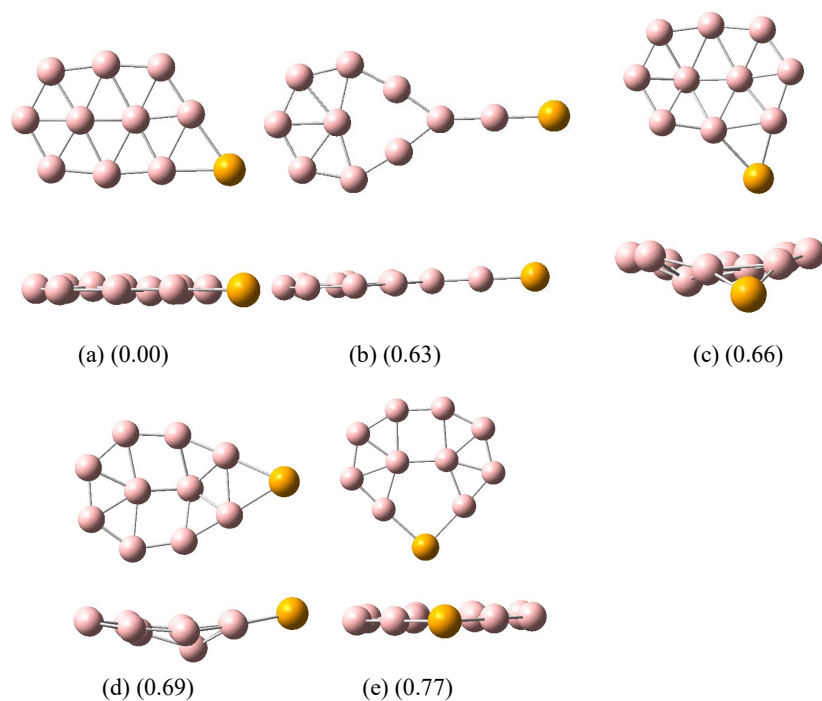


**Figure S14.** Low-lying isomers of doped boron clusters  $\text{SeB}_9^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_9^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

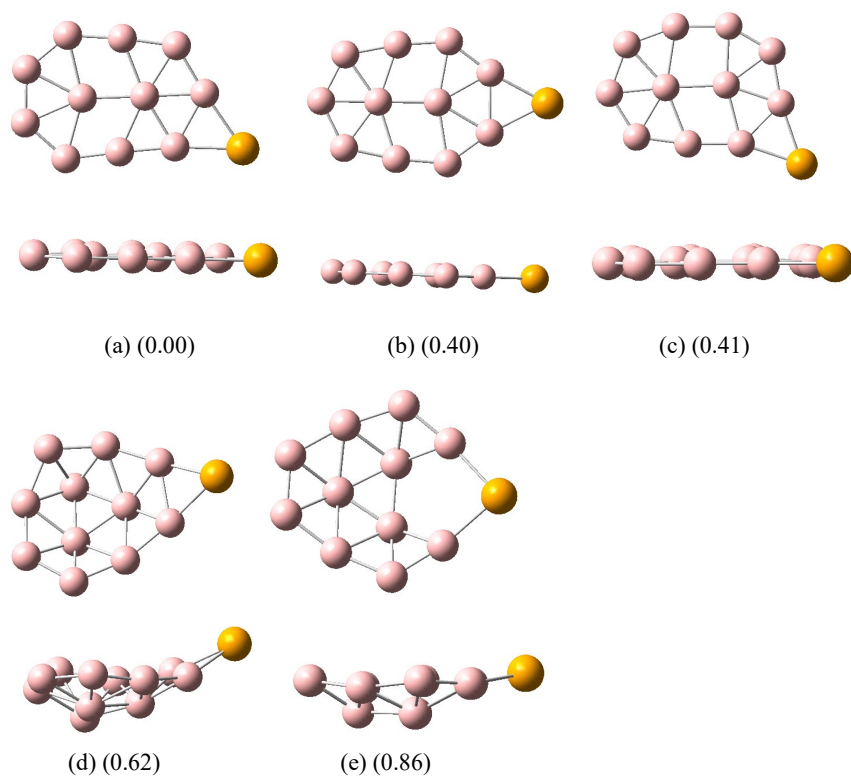




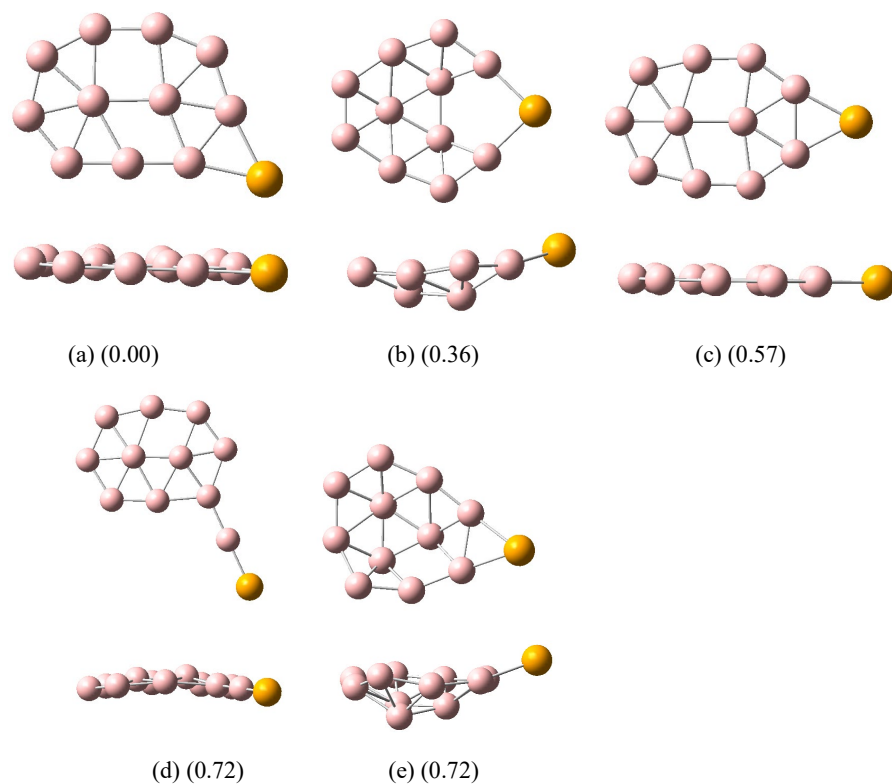
**Figure S15.** Low-lying isomers of doped boron clusters  $\text{SeB}_{10}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{10}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



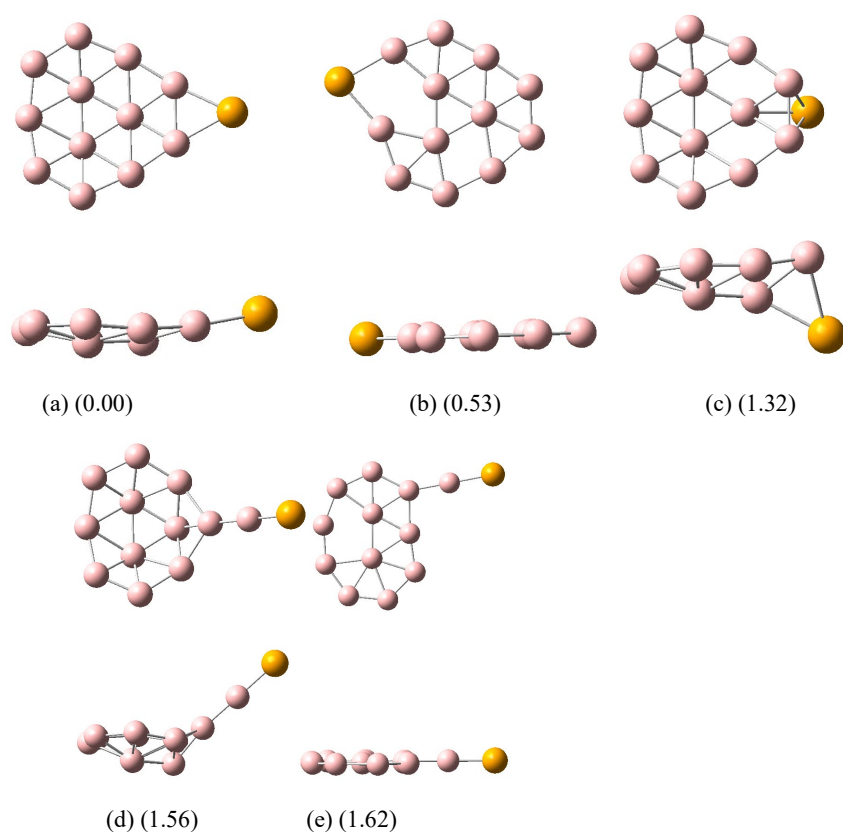
**Figure S16.** Low-lying isomers of doped boron clusters  $\text{SeB}_{10}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{10}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



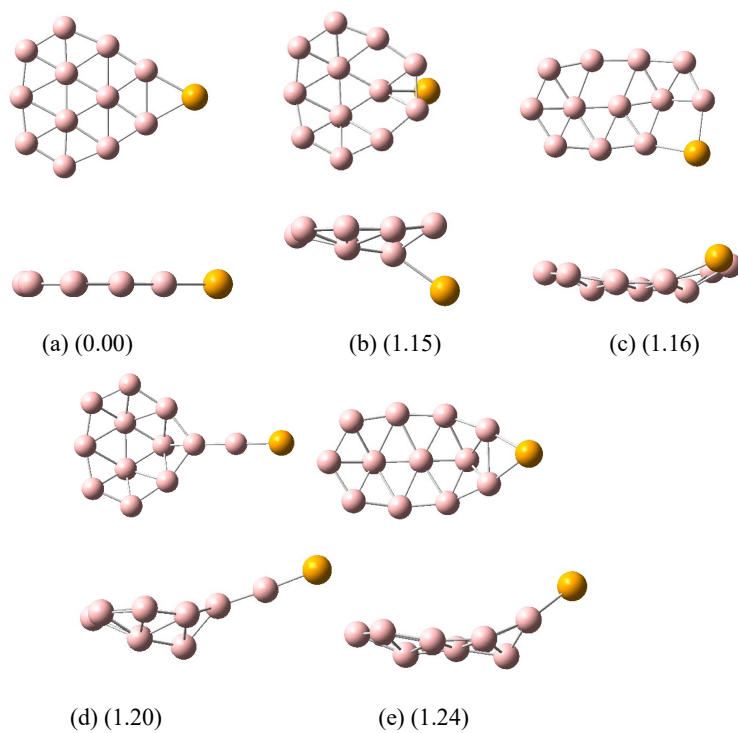
**Figure S17.** Low-lying isomers of doped boron clusters  $\text{SeB}_{11}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{11}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



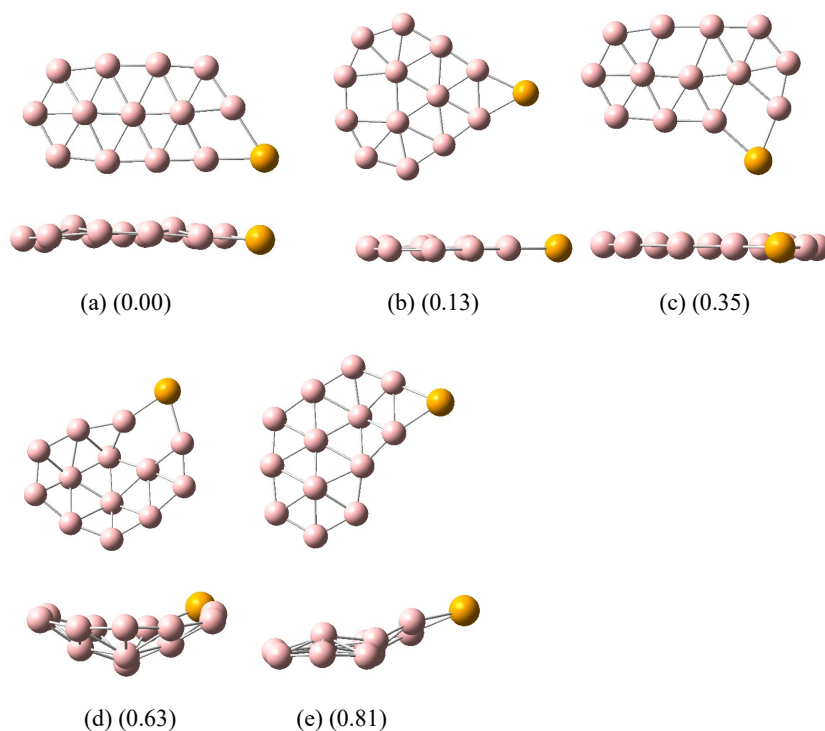
**Figure S18.** Low-lying isomers of doped boron clusters  $\text{SeB}_{11}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{11}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



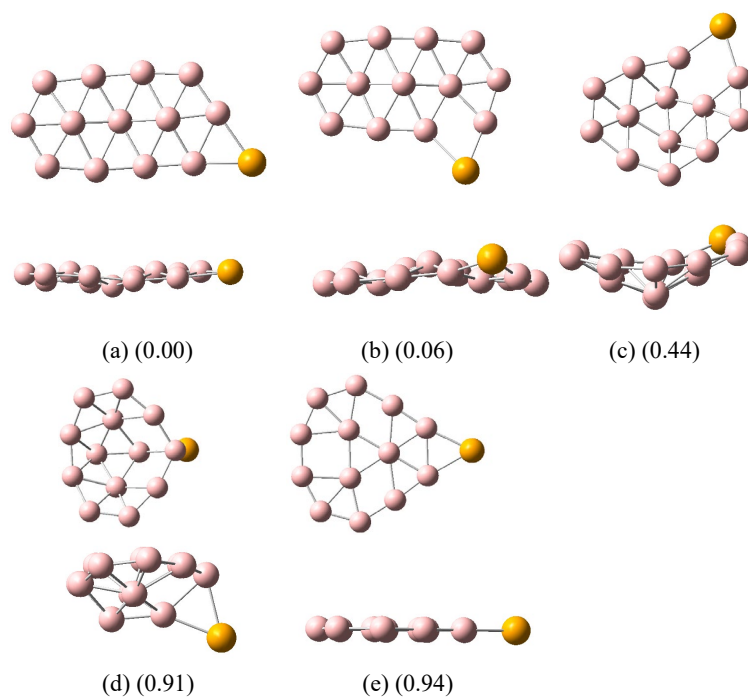
**Figure S19.** Low-lying isomers of doped boron clusters  $\text{SeB}_{12}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{12}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



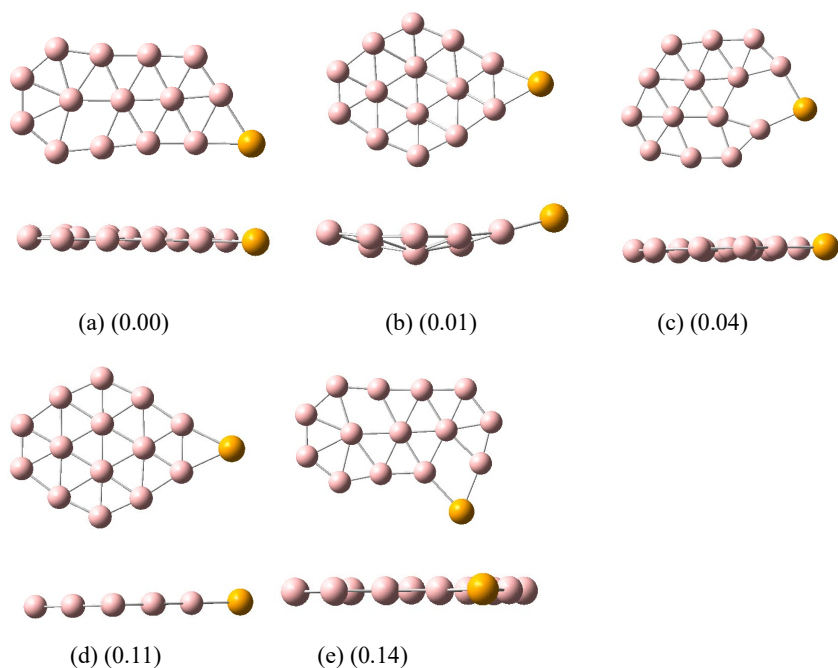
**Figure S20.** Low-lying isomers of doped boron clusters  $\text{SeB}_{12}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{12}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



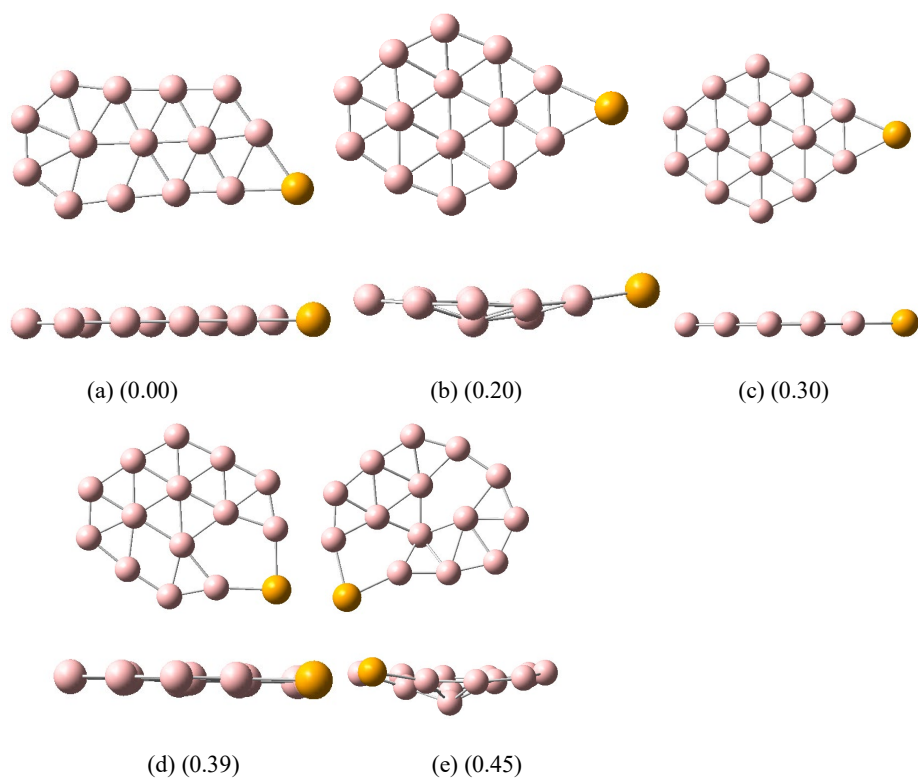
**Figure S21.** Low-lying isomers of doped boron clusters  $\text{SeB}_{13}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{13}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



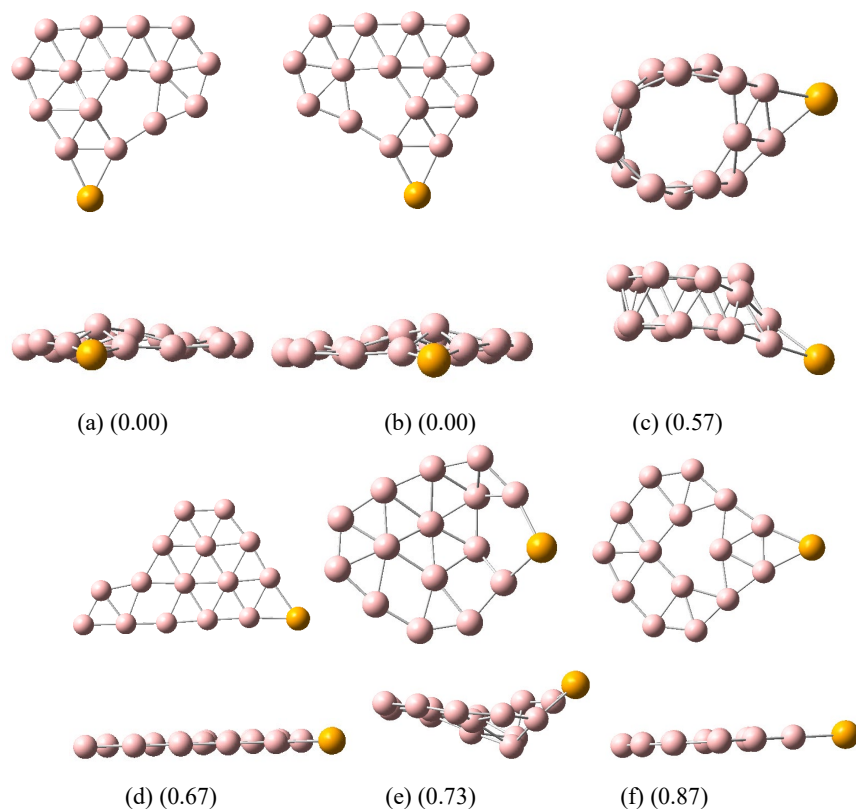
**Figure S22.** Low-lying isomers of doped boron clusters  $\text{SeB}_{13}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{13}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



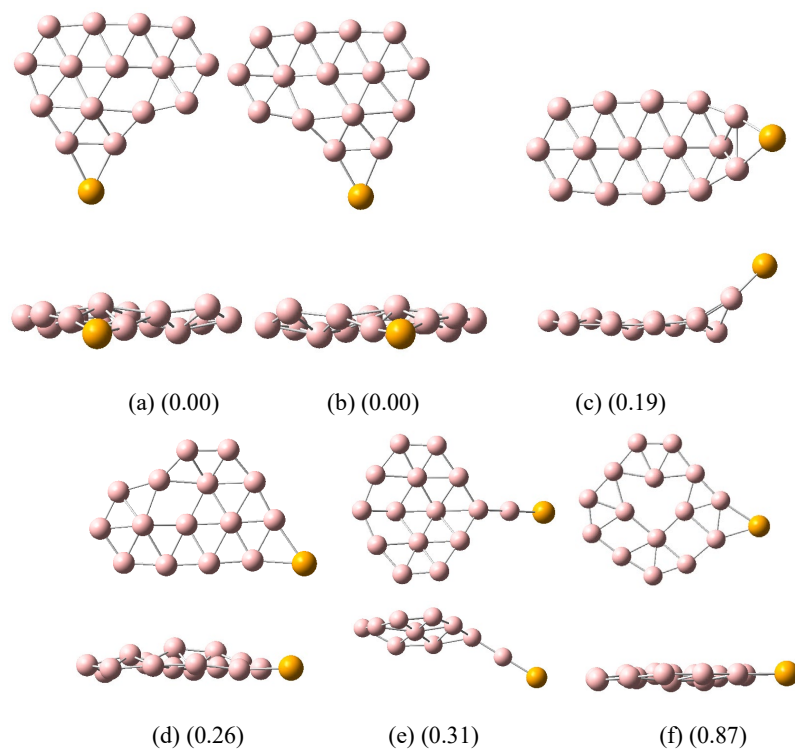
**Figure S23.** Low-lying isomers of doped boron clusters  $\text{SeB}_{14}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{14}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



**Figure S24.** Low-lying isomers of doped boron clusters  $\text{SeB}_{14}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{14}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

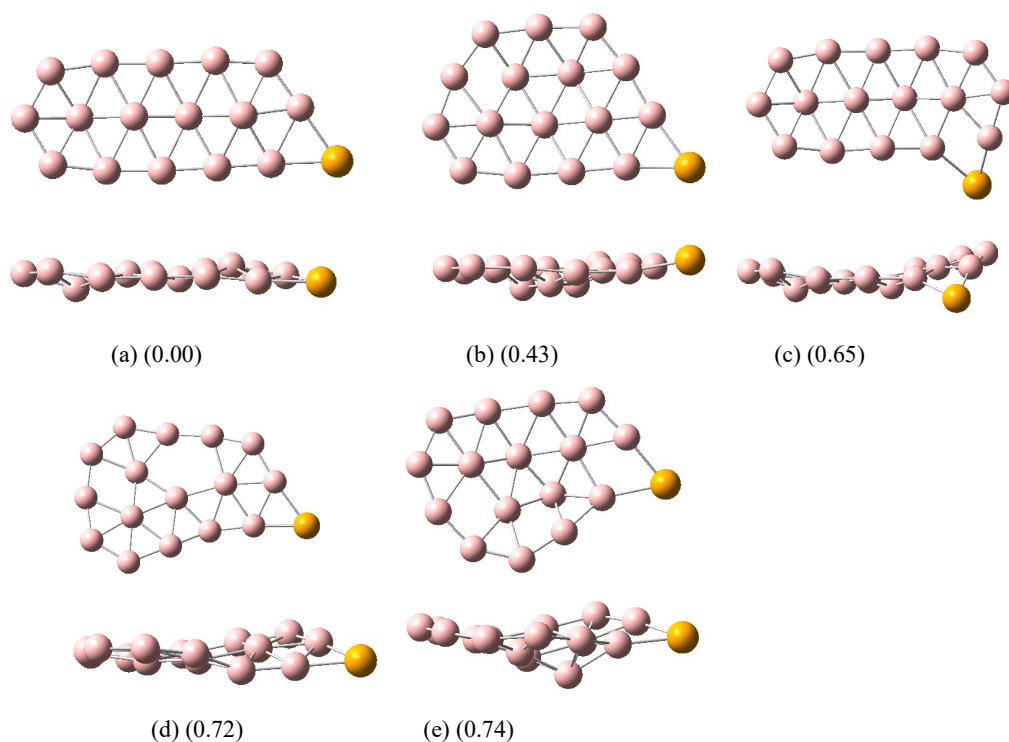


**Figure S25.** Low-lying isomers of doped boron clusters  $\text{SeB}_{15}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{15}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

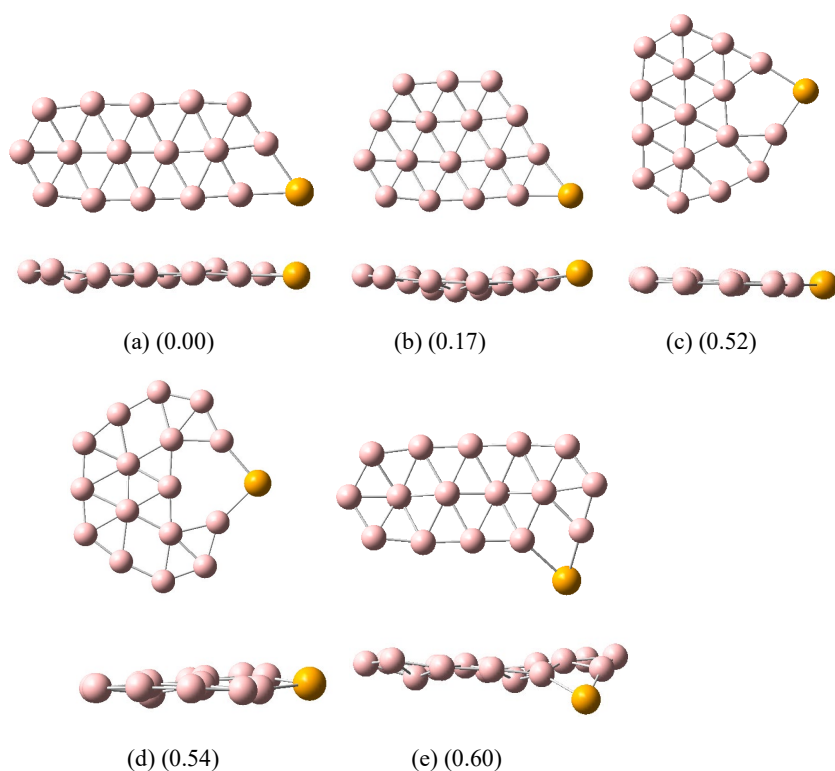


**Figure S26.** Low-lying isomers of doped boron clusters  $\text{SeB}_{15}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{15}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.

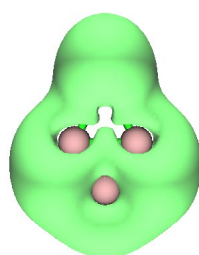




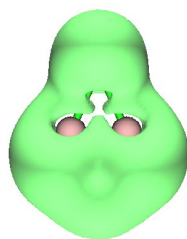
**Figure S27.** Low-lying isomers of doped boron clusters  $\text{SeB}_{16}$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{16}$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



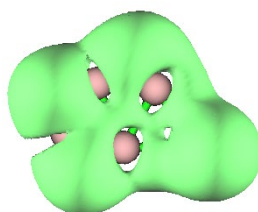
**Figure S28.** Low-lying isomers of doped boron clusters  $\text{SeB}_{16}^-$ . Values in parentheses are the relative energies (eV) of the five low-energy isomers for  $\text{SeB}_{16}^-$  at the PBE0/6-311+G\* level. The upper row is top view and the bottom row is side view.



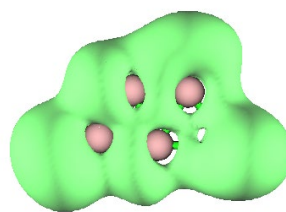
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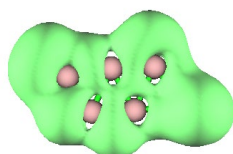
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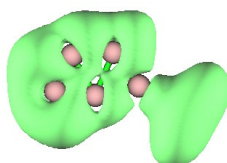
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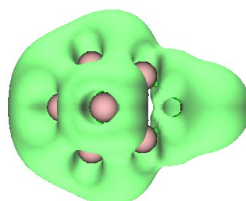
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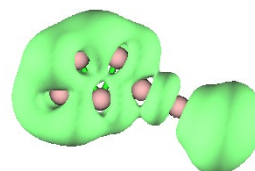
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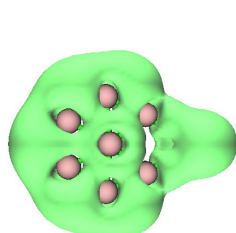
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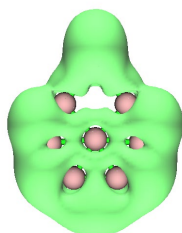
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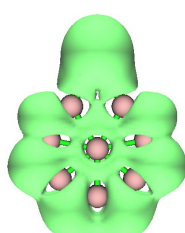
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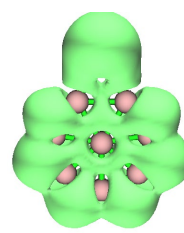
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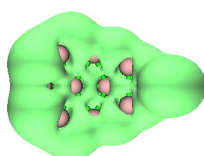
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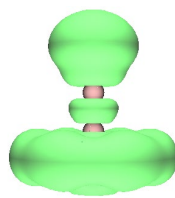
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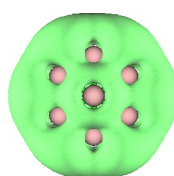
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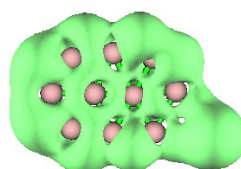
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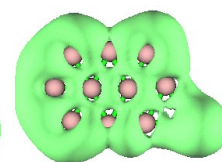
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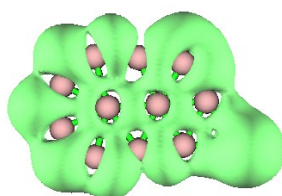
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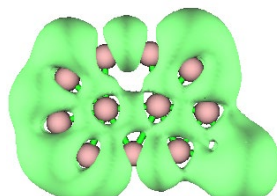
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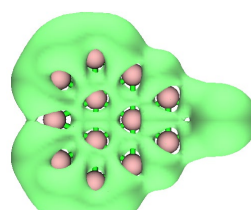
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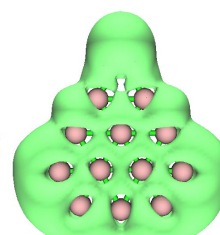
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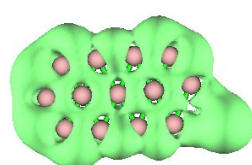
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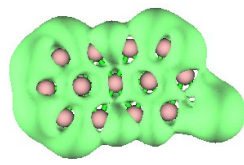
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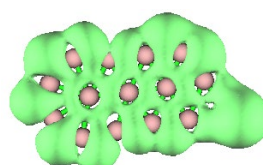
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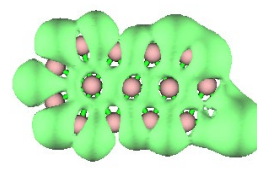
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SeB<sub>13</sub><sup>-</sup>

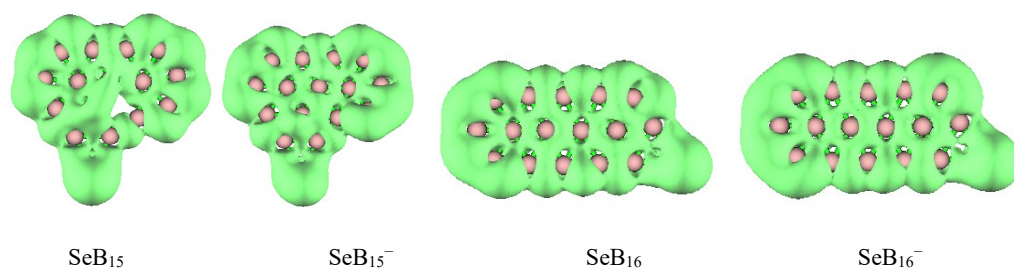


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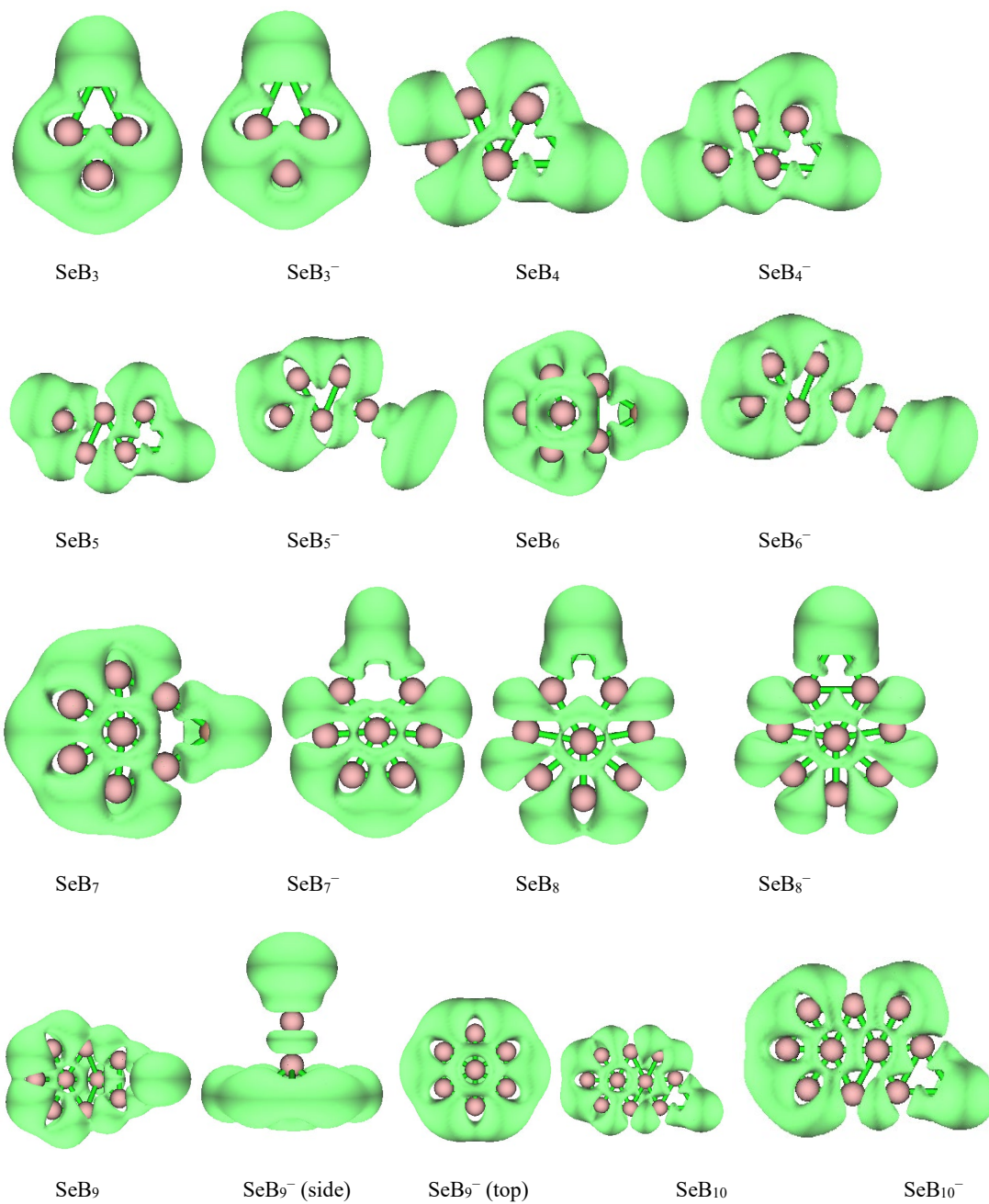


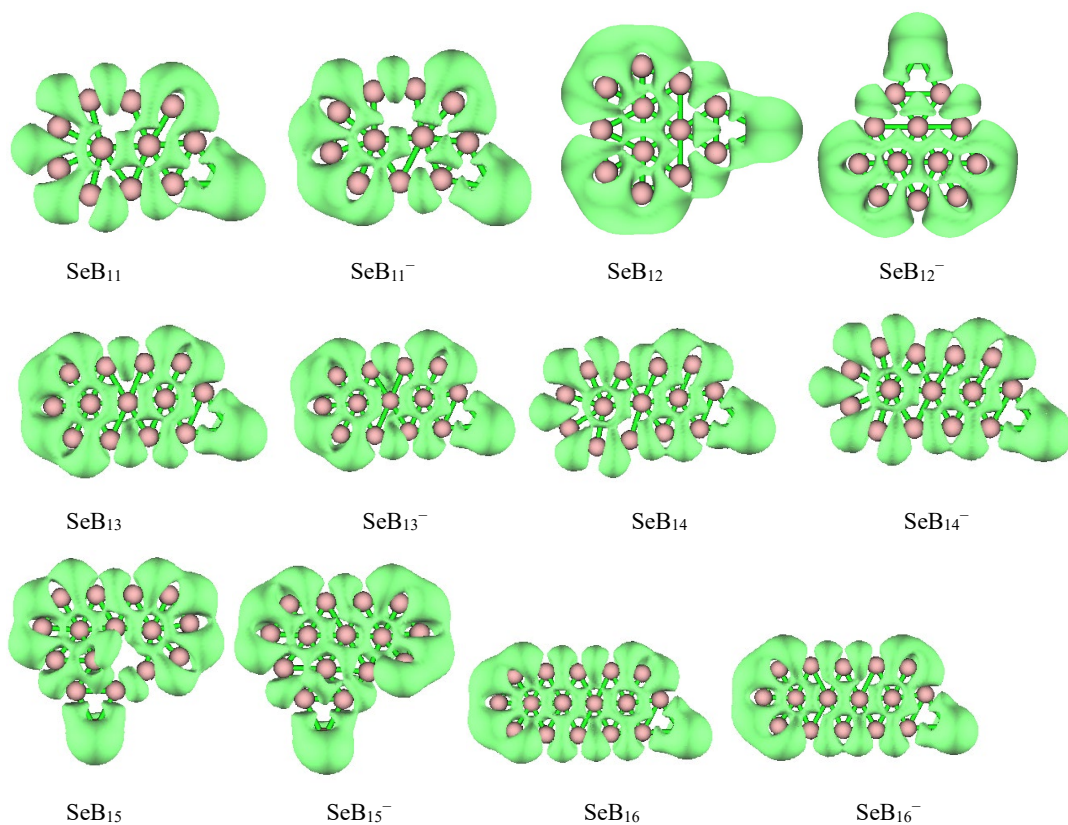
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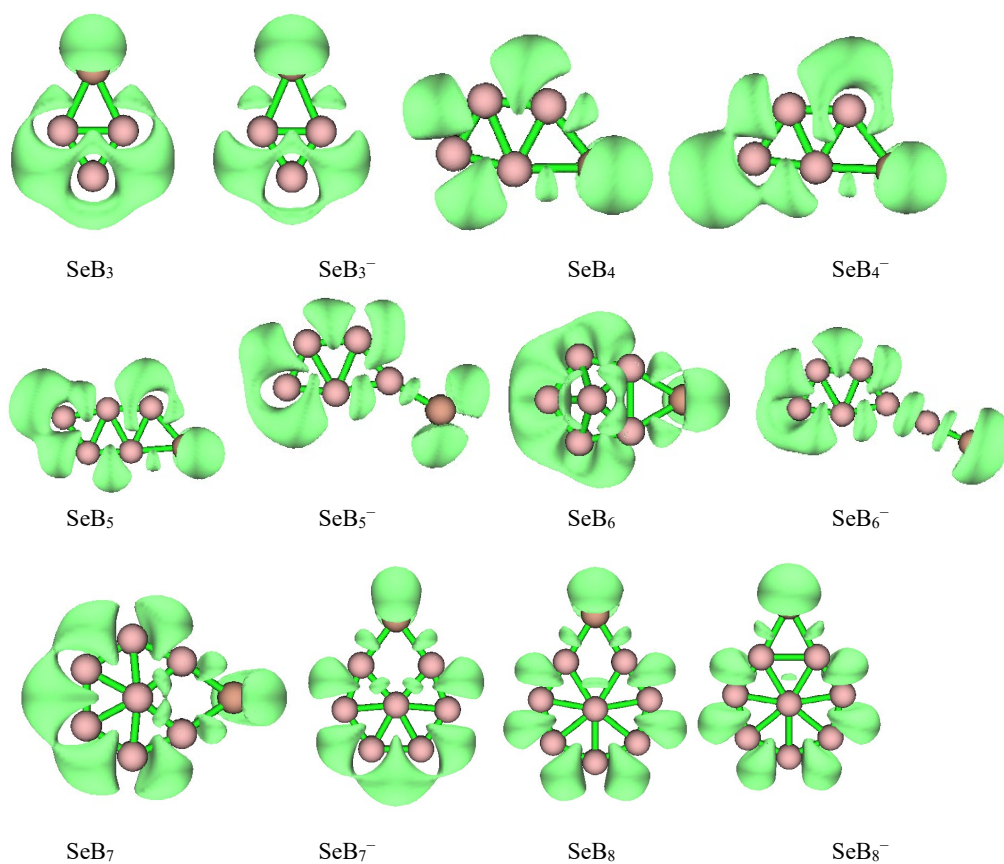


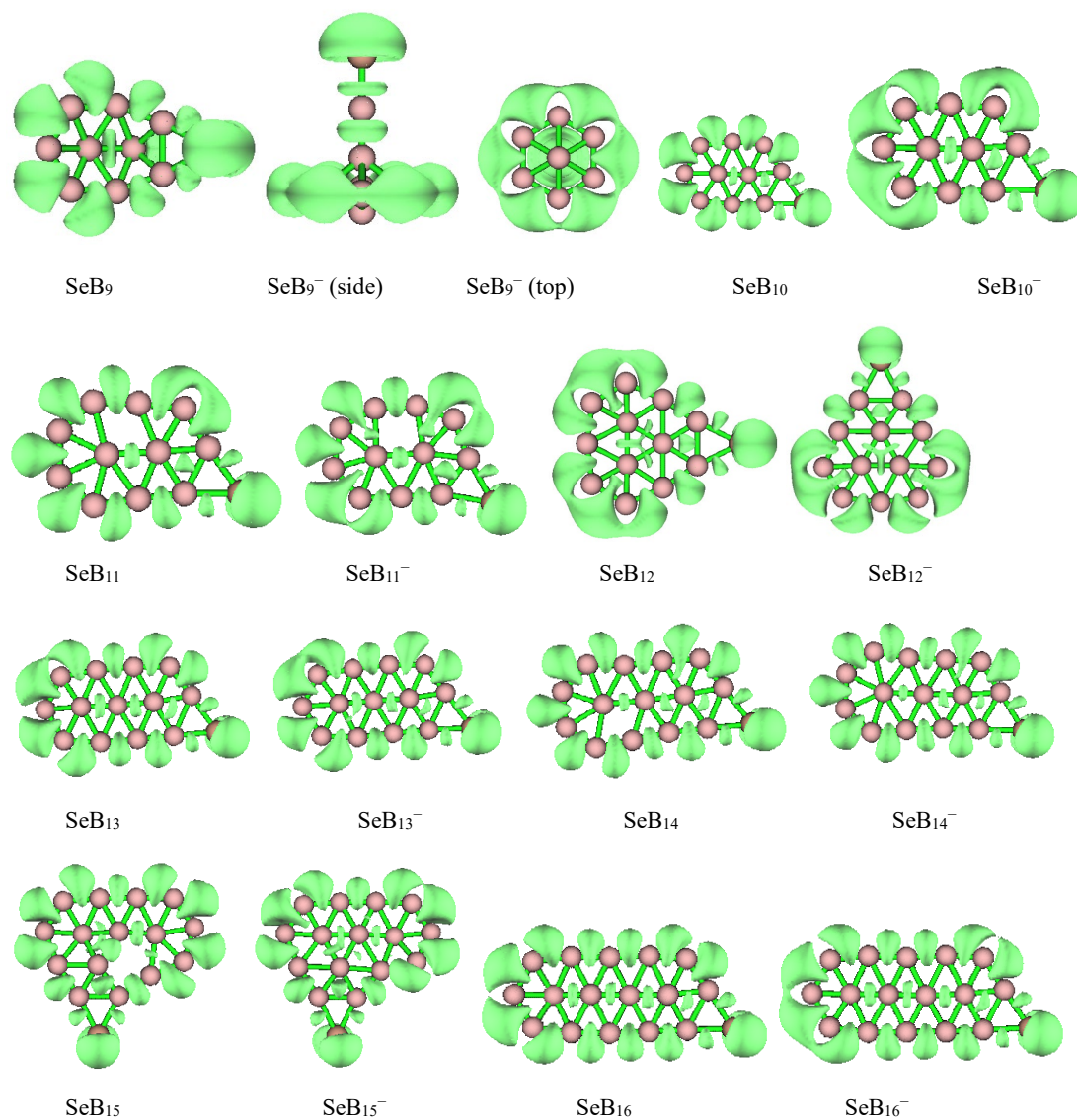
**Figure S29.** Electron localization function (ELF) with the isovalue set to 0.60.





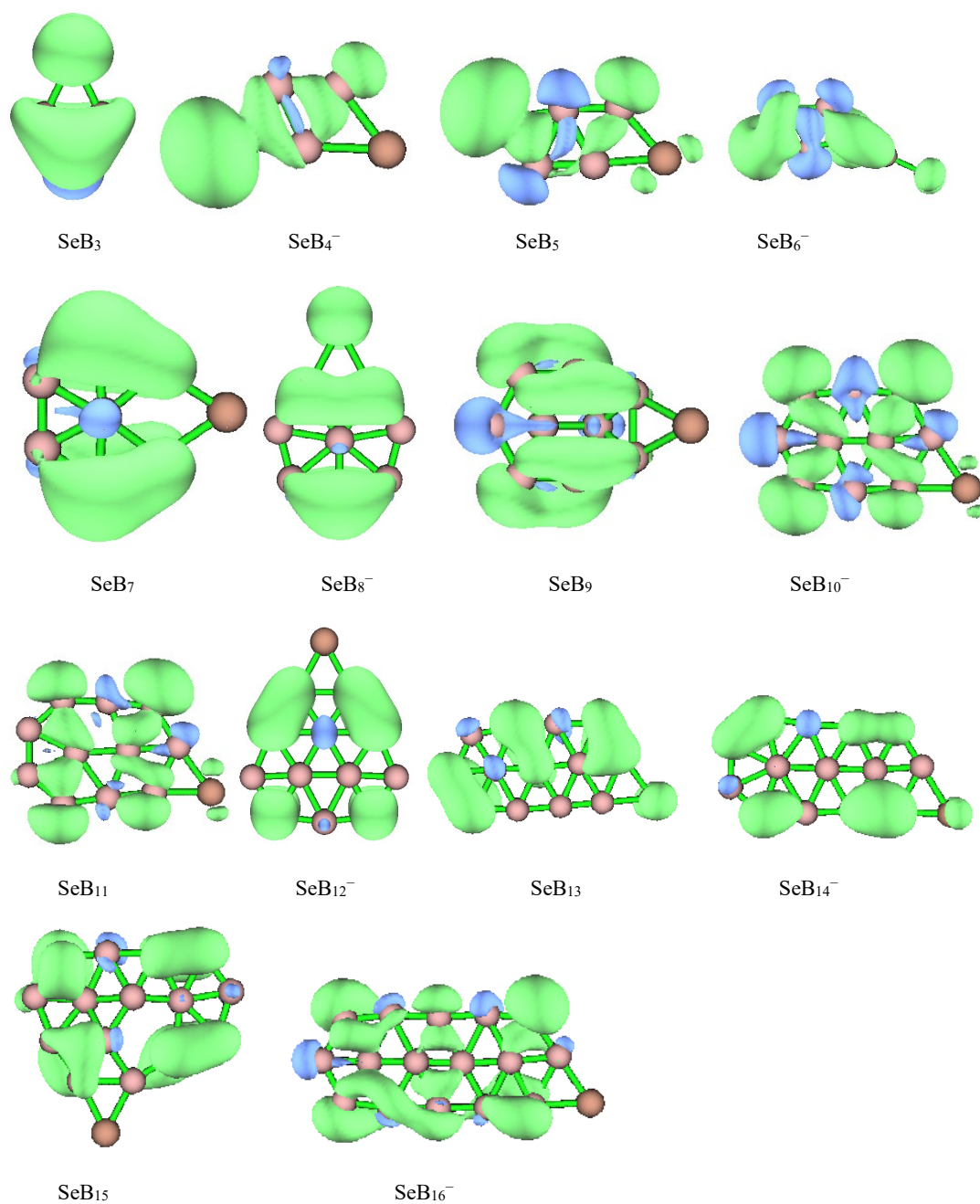
**Figure S30.** Electron localization function (ELF) with the isovalue set to 0.70.





**Figure S31.** Electron localization function (ELF) with the isovalue set to 0.80.





**Figure S32.** Spin density with the isovalue set to 0.002. Green represents a positive value (alpha electrons), and blue represents a negative value (beta electrons).