DFT Study on the Selective Complexation of B12N12 Nanocage with Alkali Metal Ions

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**Supplemental Materials**

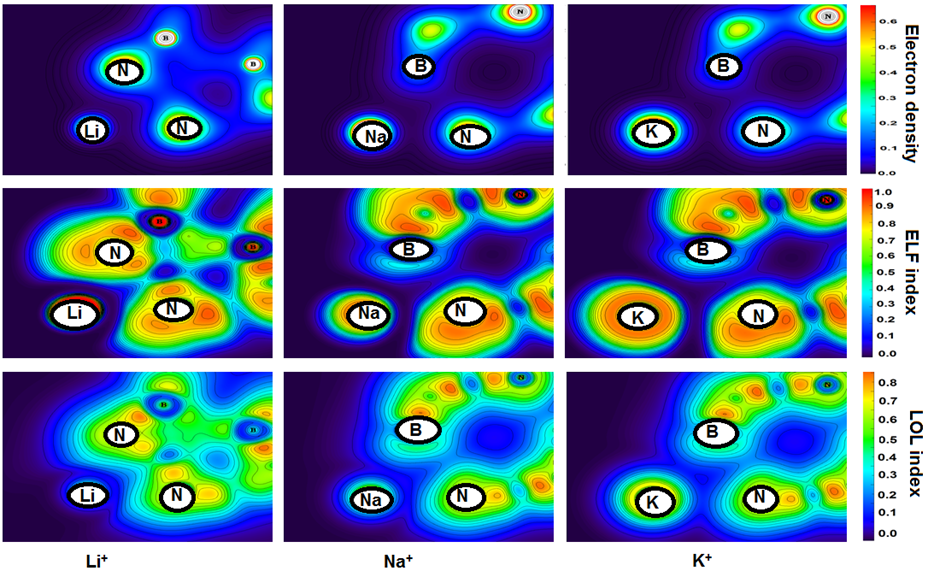


Figure S 1. Electron density, ELF and LOL plots of the ion-BN (SA) interaction in the gas phase.

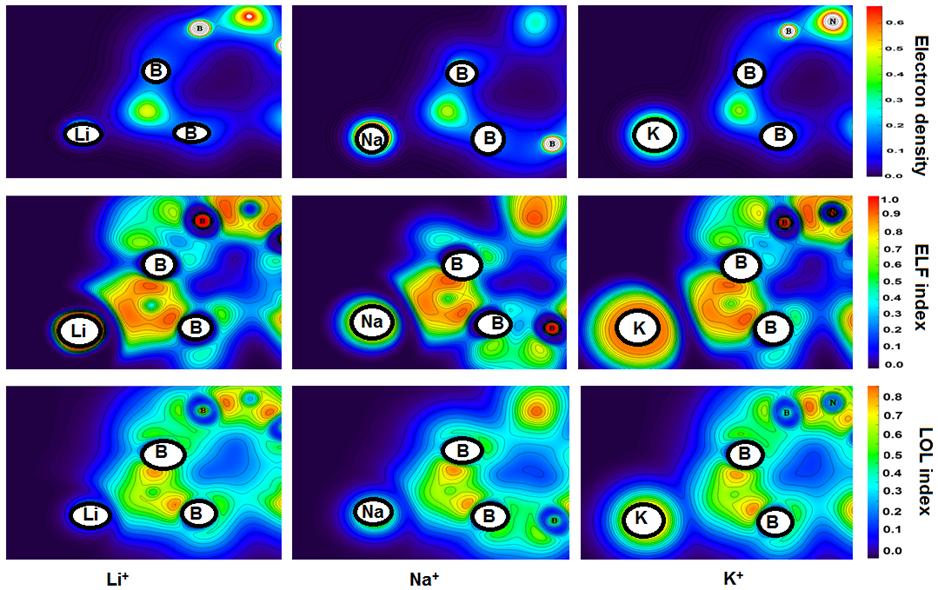


Figure S 2. Electron density, ELF and LOL plots of the ion-BN (SB) interaction in the gas phase.

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| Table S 1. Thermodynamic parameters (kJ.mol−1) of the metal ion complexes with BN in the gas phase and water. | | | | | | | | |
|  | | SA | | | | SB | | |
|  |  | ∆G | ∆E | ∆H | ∆G | | ∆E | ∆H |
| Li+ | Gas | -87.63 | -109.11 | -111.59 | -109.24 | | -130.98 | -133.46 |
| Water | 25.36 | -2.28 | -4.76 | 19.82 | | -0.02 | -2.49 |
| Na+ | Gas | -54.00 | -74.29 | -76.77 | -63.86 | | -83.12 | -85.59 |
| Water | 20.53 | -0.75 | -3.23 | 18.21 | | -1.03 | -2.41 |
| K+ | Gas | -30.92 | -50.09 | -52.57 | -35.85 | | -50.62 | -53.09 |
| Water | 14.48 | 1.95 | -0.52 | 16.70 | | 1.98 | -0.49 |
| Rb+ | Gas | -19.14 | -37.66 | -40.14 | -8.66 | | -32.96 | -35.44 |
| Water | 17.36 | 2.07 | -0.39 | 22.25 | | 0.04 | -2.43 |
| Cs+ | Gas | -13.30 | -31.29 | -33.77 | -2.97 | | -27.33 | -29.81 |
| Water | 15.09 | 1.58 | -0.88 | 15.62 | | 1.82 | -0.65 |