Supplementary data

Evolution of the structures and stabilities of boron-doped lithium cluster cations: *ab initio* and DFT studies

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Figure S1. Molecular orbitals (isovalue = 0.02 au) of $BeLi_n$, BLi_n^+ and BLi_n (n = 5-7). The superscripts indicate spin multiplicity. The continuous lines represent doubly and singly occupied orbitals for close-shell and open-shell systmes, respectively, the dotted lines correspond to unfilled states, the degenerate orbitals are arrayed parallel to each other, and the arrows indicate the α (up) and β (down) spin states.