Figure 7. The molecular orbitals (MO) and MO energy level correlation diagram of the VLi8, Li9, and single Mn2+ cationic for the lowest-energy structures calculated with PW91/LANL2DZ level in G09. Continuous lines correspond to the filled levels and the dotted lines correspond to the unfilled states. For each level, the degeneracy is marked. The surface isovalue for molecular orbital plotting is 0.02 e/Å3.

