Density functional study of Pt metal, $LiPt_2$, LiPt and Li_2Pt

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Abstract

First principles density functional theory calculations were carried out for the series of metal-rich compounds, $LiPt_2$, LiPt and Li_2Pt, and elemental Pt as a comparison to probe the bonding picture that captures the essence of their electronic structures. Our analysis shows that the 5d-electron configuration of Pt in these compounds is close to $(5d)^{10}$, and the electrons released from the Li atoms in the Li/Pt binary compounds are delocalized among the Li^+ and Pt^0 atoms through the interactions of the Pt 5d orbitals of each Pt with the Pt 6s/6p of neighboring Pt atoms and the Li 2s/2p orbitals of neighboring Li atoms. The electron counting schemes best representing the electronic structures of Pt metal, $LiPt_2$, LiPt and Li_2Pt are Pt^0 (d^{10}), $Li^+[Pt^0 (d^{10})]_2(e^-)$, $Li^+[Pt^0 (d^{10})](e^-)$ and $(Li^+)_2[Pt^0 (d^{10})](2e^-)$, respectively, and hence the Pt atoms of the Li/Pt binary compounds exist as anions.