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ELECTRONIC SUPPLEMENTARY INFORMATION

On the electrostatic nature of electrides

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For representative theoretical [Li^+(Calix[4]pyrrole)e^-] and experimental [Li^+(Cryptand-2.1.1)e^-] electride Figure S1 provides the variation of molecular electron density (MED) and molecular electrostatic potential (MESP) while moving away from the metal atom along the direction of MESP minimum. Red line indicates MESP whereas blue line gives the variation of MED. As mentioned in the article, a non-nuclear maximum in MED exists between the alkali metal and the MESP minimum corresponding to trapped electron. Both the electrides show that the electron density does not decay monotonically, rather passes through a local maximum (location of non-nuclear maximum in MED topography). The variation in MED is sharper in [Li^+(Cryptand-2.1.1)e^-] (at ~1.5 Å) compared to [Li^+(Calix[4]pyrrole)e^-] (at ~1.7 Å), which possesses relatively shallow maximum. However it can be clearly observed that the MESP in both the cases is highly positive at the location of non-nuclear maximum of MED. This is mainly due to the positive potential created by nuclear framework. MESP does not exhibit non-nuclear maximum, a theorem rigorously proven by Gadre *et al.* Thus, minimum in MESP provides the region of electron concentration. As can be observed in Figure S1, the minimum in MESP is located far away from the non-nuclear maximum of MED. A peculiar notch can be observed in the negative MESP region of [Li^+(Cryptand-2.1.1)e^-], indicating two MESP minimum separated by certain distance. Thus it can be concluded that electronic properties of electrides reveal lot of unique and intriguing features.

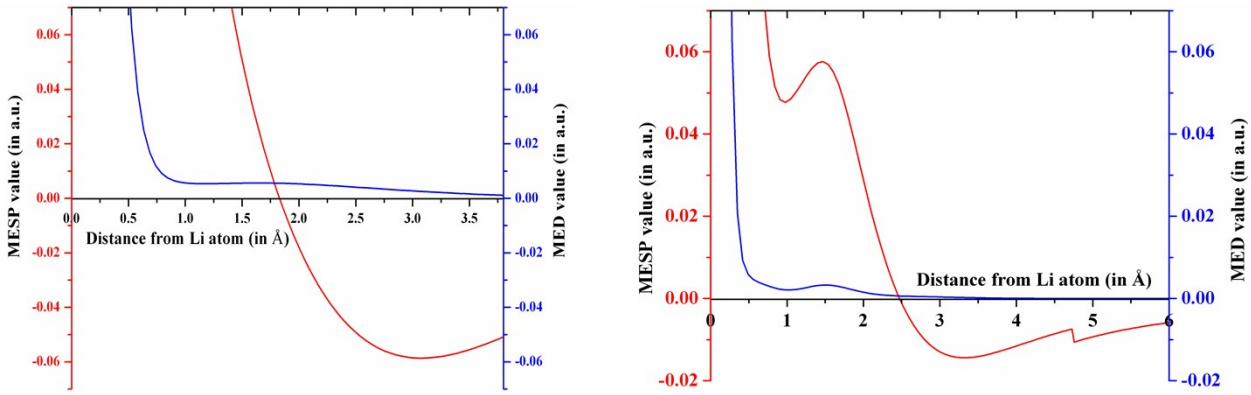

Figure S1. Plot of MED and MESP along the line joining alkali metal atom, non-nuclear maxima in MED and minimum in MESP for **(a)** Li^+(Calix[4]pyrrole)e^- and **(b)** Li^+(Cryptand-2.1.1)e^- . Alkali metal is located at origin.