The main discharge products formed at the cathode of nonaqueous Li-air batteries are known to be Li2O2 and residual Li2CO3. Recent experiments indicate that the charge transport through these materials is the main limiting factor for the battery performance. It has been also shown that the performance of the battery decreases drastically when the amount of Li2CO3 at the cathode increases with respect to Li2O2. In this work, we study the formation and transport of hole and electron polarons in Li2O2 and Li2CO3 using density functional theory (DFT) within the PBE+U approximation. For both materials, we find that the formation of polarons (both hole and electron) is stabilized with respect to the delocalized states for all physically relevant values of U. We find a much higher mobility for hole polarons than for the electron polarons, and we show that the poor charge transport in Li2CO3 compared to Li2O2 can be understood through a polaronic model for the conduction. Furthermore, the hole polaronic model in Li2O2 provides a possible explanation for the experimentally observed preferential growth direction of the films. Our results also suggest that doping is unlikely to be a viable route for improving the transport properties of Li2O2 or Li2CO3.
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