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**Organic electrodes for high rate capability Lithium-ion batteries** Y.Y. ZHANG, Y.Y. SUN, Rensselaer Polytechnic Institute, S.X. DU, H.J. GAO, Institute of Physics, Chinese Academy of Sciences, S.B. ZHANG, Rensselaer Polytechnic Institute — Lithium-ion batteries (LIBs) for power-intensive applications such as in electric vehicles require high discharge rate, i.e., high Li diffusion rate (or low Li diffusion barrier) in electrode and electrolyte materials. Based on first-principles calculations, we found that organic salt, di-lithium terephthalate (Li2TPA), a promising anode material recently tested in experiment, could have high rate capability. We further predict that di-potassium terephthalate (K2TPA) could exhibit even lower Li diffusion barrier. The calculated Li diffusion barrier in fully lithiated K2TPA is only 150 meV, which yields Li diffusion rate orders of magnitude higher than that in Li-intercalated graphite at room temperature. The calculated anode voltage vs metal lithium and specific energy density are 0.62 V and 209 mAh/g, respectively. In addition, the volume change of K2TPA in charging/discharging is only 5%, much smaller than that in Li-intercalated graphite. These unique advantages call for further investigation of the organic salts, both the TPA-based and beyond, for power-intensive LIB applications either as anode or cathode materials.

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