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Insight into the limitation of intrinsic capacity of cathode materials for Li-ion batteries PENG ZHANG, WEI SUHUAI, Beijing Computational Science Res Ctr — To increase the capacity of Li-ion batteries (LIBs), development of new cathode materials that can accommodate more than one Li ions per formula unit (f.u.) is highly required. However, one critical point is that the nominal amount of Li ions stored in cathode materials may not equal to their practical capacities, i.e. there may be a certain amount of inert Li ions that cannot be reversibly used. Based on the DFT calculations, we identify a general rule of intrinsic capacity limitation for LIB cathode materials, especially for those with more than one Li ions per f.u. in their hosts. Based on the rule, it is easy to understand why only one Li ion in many Li-rich cathode materials, e.g. Li_2FeSiO_4, could be reversibly used. Thus, this rule implies a guideline for future cathode design.

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