

Fractional and integer stages of lithium ion-graphite systems. The role of electrostatic and elastic contributions.

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Supplementary Information

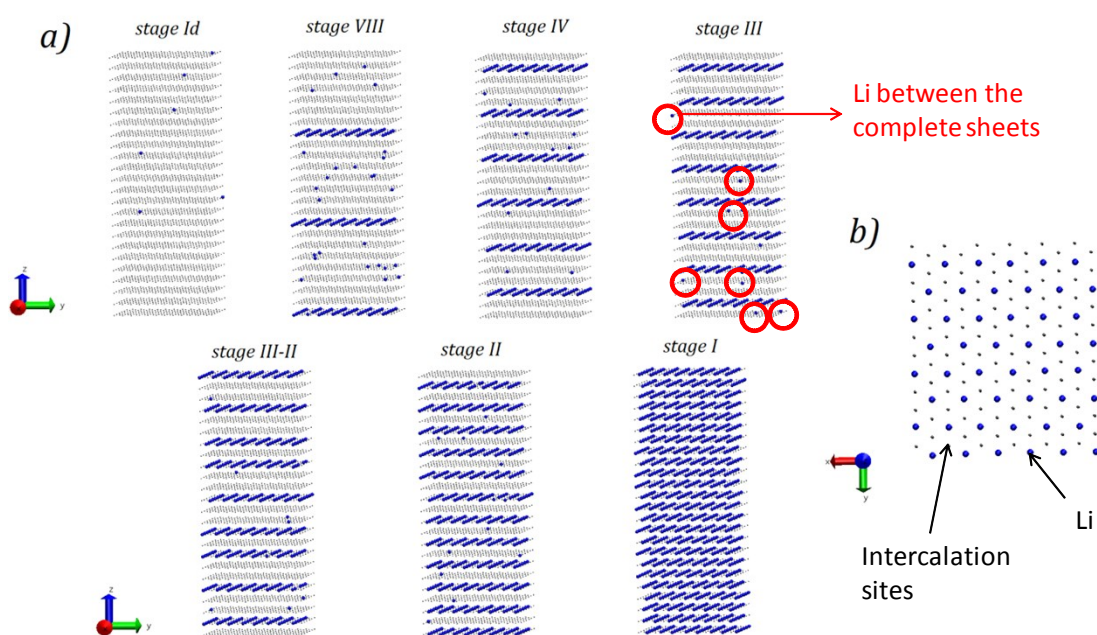


Figure S1: a) Snapshots from Grand Canonical Monte Carlo simulations, showing the different structures obtained. The gray spheres correspond to empty intercalation sites and the blue ones to Li atoms. For simplicity C atoms are not shown. Note the presence of inserted Li-ions between filled Li-ion layers. These kind of inserted ions are practically absent in simulations that do not consider elastic effects. b) Snapshot of a top view of the simulation box, showing the $\sqrt{3} \times \sqrt{3}$ Li structure in a given plane.