A first-principle approach for electrochemical stress and strain developed on electrode materials for Li-ion batteries.

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Although Lithium-ion battery has great contributions to the emergence of electronics industry, it is still far away to satisfy the major challenges that require more energy stored for a long lifespan. One of these challenges is to increase the stability of the electrode material upon the electrochemical cycling. Indeed, during the charge discharge process the electrode material is subjected to volume variations inducing mechanical stress, so that it can result either in cracking when the stress is too important (out of elastic regime) or in phase transition when the material becomes mechanically unstable (following the Born conditions). In that context, recent experimental works have been devoted to measure *insitu* the electrochemical stress and strain and their influence on the electrochemical properties of electrode material[1–3]. We develop a methodological approach based on first-principles DFT calculations to access electrochemical stress and strain and their influence on the electrochemical performance on the electrode. In light of this concept we revisit the mechanisms taking place during the cycling of the spinel $LiMn_2O_4$ and the Layered $LiMnO_2$.

References:

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