Article title: Classical molecular dynamics and quantum abs-initio studies on lithium-intercalation in interconnected hollow spherical nano-spheres of amorphous Silicon

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Abstract:
A high concentration of lithium, corresponding to charge capacity of ~4200 mAh/g, can be intercalated in silicon. Unfortunately, due to high intercalation strain leading to fracture and consequent poor cyclability, silicon cannot be used as anode in lithium ion batteries. But recently interconnected hollow nano-spheres of amorphous silicon have been found to exhibit high cyclability. The absence of fracture upon lithiation and the high cyclability has been attributed to reduction in intercalation stress due to hollow spherical geometry of the silicon nano-particles. The present work argues that the hollow spherical geometry alone cannot ensure the absence of fracture. Using classical molecular dynamics and density functional theory based simulations; satisfactory explanation to the absence of fracture has been explored at the atomic scale.