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Theoretical investigation of C_3N monolayer as anode material for Li/Na-ion batteries.

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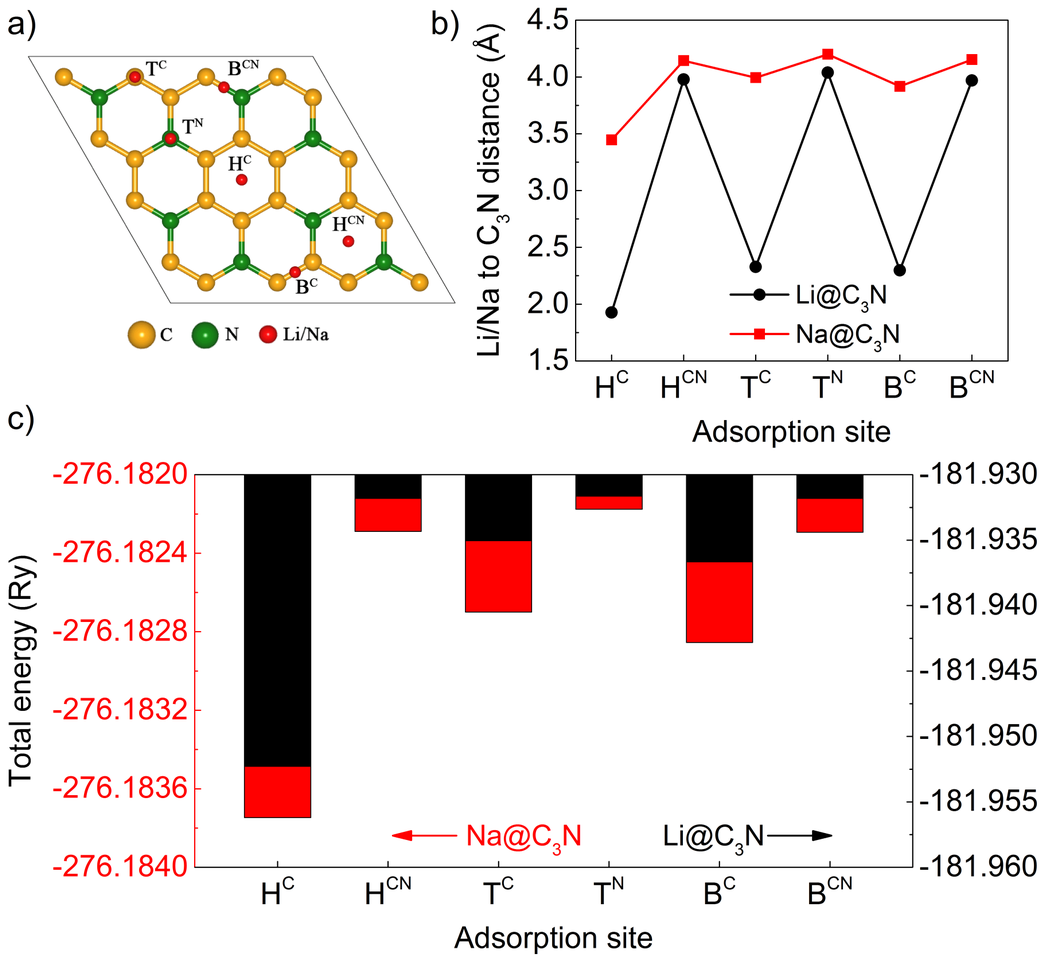
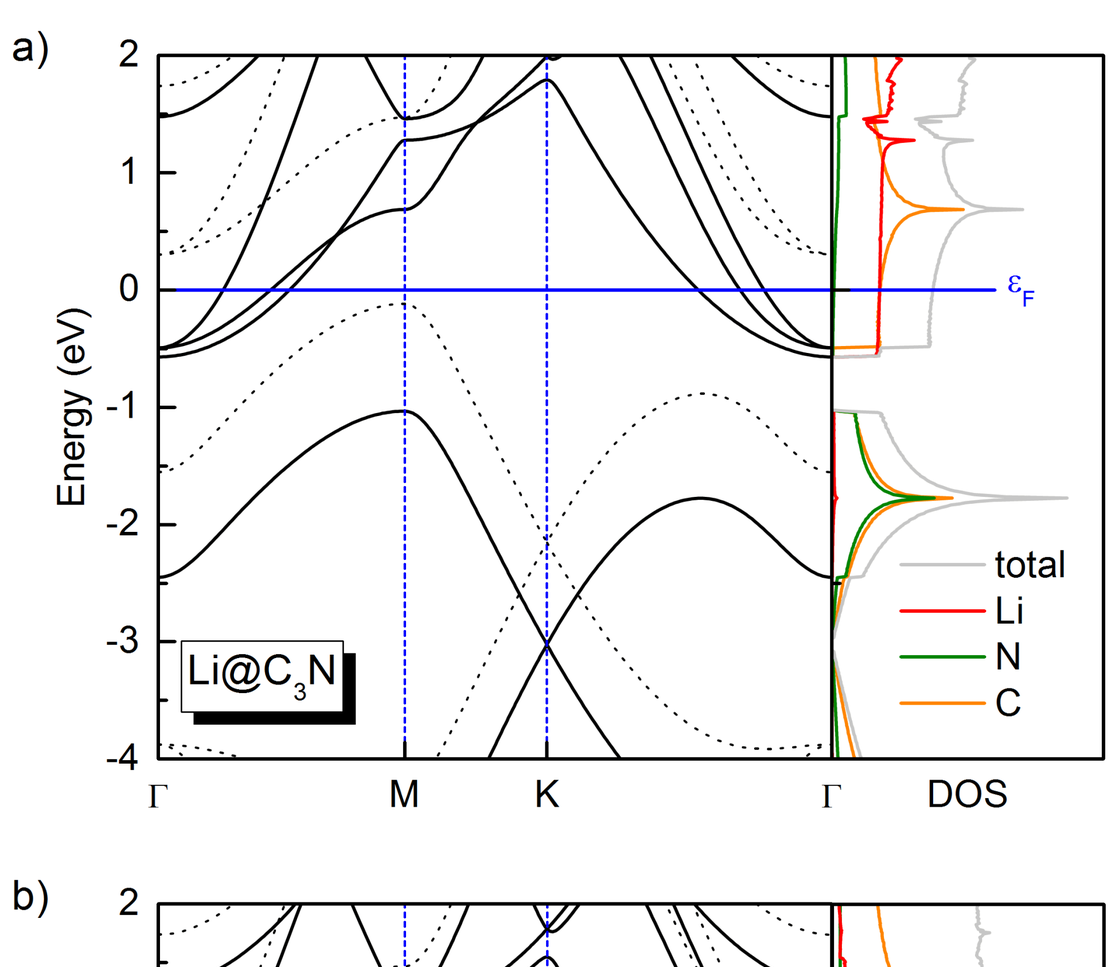
Next-generation renewable energy technology demands electrode materials with suitable structural, electronic, and mechanical properties. Based on the ab-initio analysis of 2D carbon and nitrogen material, we found that the C_3N monolayer is one of the promising candidates for useas an anode material in Li- and Na-ion batteries. In particular, we performed first-principles calculations to investigate the geometric structure, binding energies and band structure variationsof C_3N monolayer after surface ion adsorption. We find that the Li and Na atoms prefer to stay in the hollow site among hexagonal carbon ring and the second energetically most favorable site is the bridge site over the C-C bond. Moreover, our results demonstrate that after lithiation and sodiation, a semiconductor-to-metal transition is observed in C_3N monolayer.





First-principles calculations-based on density functional theory has been carried out to investigate the adsorption of Li and Na atoms on a C_3N monolayer to explore its potential applications as anode material in Li- and Na-ion rechargeable battery. Our calculations showed, that the optimal adsorption sites of Li/Na ions on the C_3N is the hollow site above the center of the carbon hexagon. A transition from semiconducting to metallic state upon lithiation/sodiation and theoretical capacity of 267.82 mAh g^{-1} reveal the potential of C_3N monolayer to be an appropriate for use as anode material.