

Theoretical Investigation of a Tetrazine Based Covalent Organic Framework as a Promising Anode Material for Sodium/Calcium Ion Batteries

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Supporting Information

S1. Electron localization function (ELF) plots of bilayer TZA at (a) (100) and (b) (010) cutoff planes, respectively .

S2. Electronic band structure plot of bilayer TZACOF using HSE06 functional.

S3. Top views of the bilayer TZACOF after the adsorption of (a) sodium and (b) calcium atom.

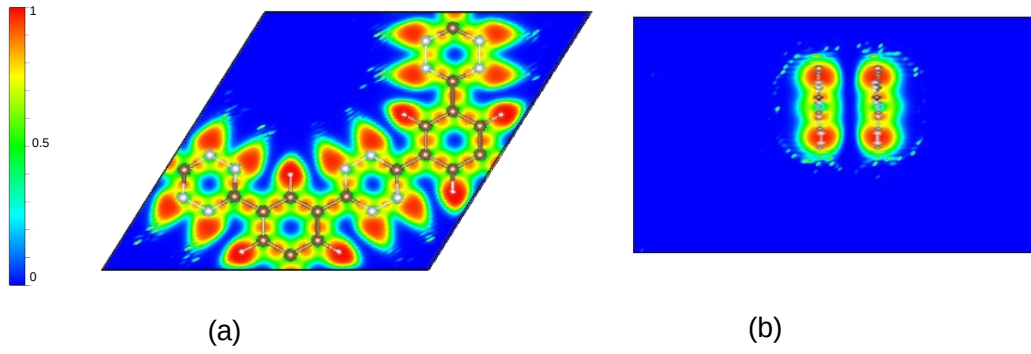


Figure 1: Electron localization function (ELF) plots of bilayer TZACOF at (a) (100) and (b) (010) cutoff planes, respectively

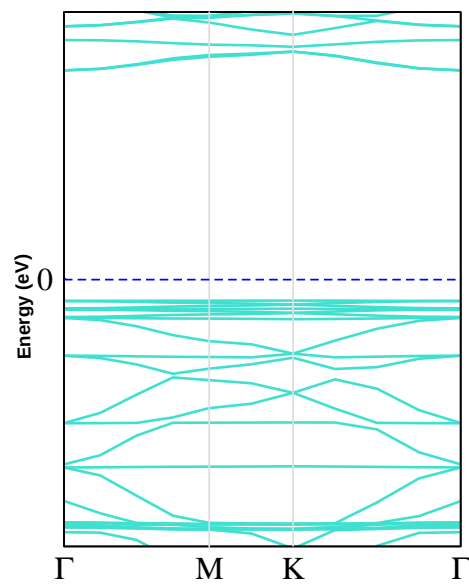


Figure 2: Electronic band structure plot of bilayer TZACOF using HSE06 functional

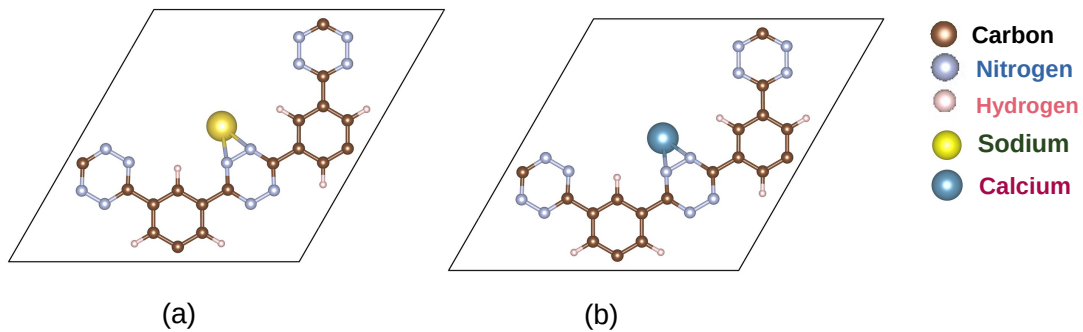


Figure 3: Top views of the bilayer TZACOF after the adsorption of (a) sodium and (b) calcium atom.