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Ab Initio Studies of Organic Electrodes for Li and Na Ion Batteries Based on Tetracyanoethylene

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Abstract : Organic electrodes are a way to achieve high rate (high power) and environment-friendly batteries. We present a computational density functional theory study of Li and Na storage in tetracyanoethylene based molecular and crystalline materials. Up to five Li and Na atoms can be stored on TCNE chemisorbed on doped graphene (corresponding to ~1000 mAh/gTCNE), with binding energies stronger than cohesive energies of the Li and Na metals by 1-2 eV. TCNE has been experimentally shown to form a crystalline material with Li with stoichiometry Li-TCNE. We confirm this computationally and also predict that a similar crystal based of Na-TCNE is also stable. These crystalline materials have well defined channels for facile Li or Na ion insertion and diffusion. Specifically, Li and Na binding energies in Li-TCNE and Na-TCNE crystals are about 1.5 eV and stronger than the cohesive energy of Li and Na, respectively. TCNE immobilized on conducting graphene-based substrates and Li/Na-TCNE crystals could therefore become efficient anode materials for organic Li and Na ion batteries, with which it should also be possible to avoid reduction of common battery electrolytes.

Keywords : organic ion batteries, tetracyanoethylene, cohesive energies, electrolytes
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