First-Principle Modeling Approach Towards Molecular Design of Electrode Materials Candidates for Lithium Ion Battery Applications

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Abstract

Energy storage technology is a critical factor for sustainable energy supply that will meet our growing energy demand from portable electrical devices to large electrical grids. To date, efforts to develop applicable energy storage systems have mostly focused on electrochemical devices, particularly lithium ion batteries. Despites their high energies and charge storage densities, they have been suffered from their poor power densities. It has been recently reported that carbon nanotube (CNT) based electrode materials in molecular levels could improve their power densities arising from their characteristics such as high electron conductivity, high electrochemically active surface areas. In addition, it is expected that the transport of lithium ions can be enhanced due to relatively short diffusion paths. Although CNT based electrode materials have therefore tremendously attracted as promising electrode candidates, systematic investigation of the performance of CNT based electrode materials has not been reported so far. Herein, we have employed the First-Principles Modeling approach such as density functional theory (DFT) method to study the redox potentials of CNT based electrode material candidates. Our investigation has aimed to identify the relationship of the structure electrode materials with the performance.