

527e Lithium-Ion Conducting Channels for Solid State Lithium Ion Batteries

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The crystalline structure and self-assembly characteristics of di-lithium phthalocyanine (Li₂Pc) as well as its properties as ion conductor in an electrochemical cell, where Li₂Pc is used as a solid state electrolyte and diffusion of lithium ions from the electrolyte into a pyrite (100) surface have been recently analyzed using molecular dynamics simulations. Since lithium ions diffuse from the electrolyte to the electrode, a continuous ion conducting channel through the interface is essential for fast ion transport. The systems consist of a 5-layer slab of a pyrite (100) surface in contact with multilayers of Li₂Pc located in a tetragonal unit cell, which is subjected to periodic boundary conditions. We first use molecular dynamics simulations to study such solid-solid interface with the external electric field driven force for lithium ions and analyze the possible lithium ion transport pathway. Then the continuity of such pathways is examined by investigating the electrostatic potential of selected molecular systems.