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First-Principles Study of Multilayer Lithium and Graphene Compounds for Battery Applications ALPER BULDUM, GULCIN TETIKER, Department of Physics, The University of Akron, Akron, OH — Recently, graphene and graphene based materials have attracted great interest for energy storage applications such as rechargable Li-ion batteries and supercapacitors. However, recent experiments showed that these materials may have different electrochemical mechanism compared to graphite. Porosity and presence of single or few layers of graphene play important roles in carbon based anode materials in lithium ion batteries. In this work, a study of different multilayer lithium-graphene compounds is performed using first-principles density-functional theory(DFT). Relaxed structures are determined, adsorption energies, density of states and charge density are calculated. Possible multilayer structures for energy storage are discussed.

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