

嵌锂石墨充电机制的 **abinitio** 和 **DFT** 理论研究

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收稿日期 修回日期 网络版发布日期 接受日期

**摘要** 用 **ab initio/HFt DFT/B3LYP** 方法探究了在锂离子二次电池中锂离子在石墨负电极材料里可逆脱过程。理论计算结果表明, 嵌锂石墨 **LIG** 充放电机制是锂在石墨 碳层间可闹乱子嵌脱, 同时伴随着锂与碳层间发生电荷连续转移和碳层堆积方式改变的协同过程; 计算结果也明确证实, 嵌锂石墨嵌入脱出锂离子的过程就是锂离子 二次电池储存与释放能量的过程, 提出的嵌锂石墨充放电机制较好地丰富了固体电 解质相界面 **SEI** 机理和单电子还原机理。

**关键词** [从头计算法](#) [锂离子](#) [电池](#) [石墨](#) [还原](#)

分类号 [0641](#)

## Ab initio and DFT Study of the Charging-discharging Mechanism of Lithium Intercalated Graphite

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**Abstract** Several small models of graphite, lithium intercalated graphite (LIG) and lithium have been calculated at the **ab initio/HF** and **DFT/B3LYP** levels with the 6-31G and 6-31G-\* basis sets to explore the charging-discharging mechanism of **LIG** as a negative electrode in the secondary lithium battery. The obtained results demonstrate that, whilst lithium enters and leaves the graphite lattices reversibly, the continuous charge transfer between lithium and the graphite layers synchronizes with the shift of the graphite layer stacking sequences between the **AB** type and the **AA** type. Additionally, the processes of the lithium intercalation into and deintercalation out of graphite lattices are essentially that the secondary lithium battery deposits and releases the electric energy, respectively. The above charging-discharging mechanism of **LIG** enriches the **SEI** (solid electrolyte interphase) mechanism and single electron reduction mechanism of lithium into graphite very well.

**Key words** [AB INITIO CALCULATION](#) [LITHIUM ION](#) [BATTERIES](#) [GRAPHITE](#) [REDUCTION](#)

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