

锂在共轭双键高分子中的电化学嵌入反应 II: 锂在聚吡咯中嵌入反应的量子化学研究

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摘要 本文用量子化学CNDO/2方案计算,取文献中吡咯骨架原子的结构参数,再优化锂嵌入聚吡咯的几何参数.

结果表明不管是Li⁺离子还是中性Li原子,嵌入单个吡咯上还是嵌入两个吡咯之间,

它与吡咯环四个碳原子平面的距离都为0.210到0.216nm.且锂与碳原子键合,形成多中心键,锂嵌入聚吡咯后,

固有的Ca=C_s双键的键级和键能明显减弱.这与前一报中发现IR谱的1560cm⁻¹吸收峰消失相一致.

锂正离子嵌入聚吡咯后,使吡咯的前沿π*空轨道的能量由正变为负值,而成为电子接受体(正极).

遍及全部聚吡咯的π*LUMO和HOMO使得聚吡咯呈现导电性能.

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The electrochemical intercalation reaction of lithium in polymer with conjugated double bonds II quantum chemical calculation for electrochemical intercalation of Li into polypyrrole

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Abstract CNDO/2 calcs. showed that for either a Li atom or Li ion intercalated into or between the pyrrole rings, the distance between Li and pyrrole was 0.210-0.216 nm. The intercalated Li formed a polycenter bond with the C atoms. The bond order and bond energy of C:C in pyrrole decreased after intercalation, which was consistent with the disappearance of the IR absorption band at 1560 cm⁻¹. When Li⁺ was intercalated into a polypyrrole (I) electrode, the LUMO energy of pyrrole changed from pos. to neg. to become an electron acceptor capable of accepting electrons from the Li electrode of the cell. The good conductivity of I was due to the delocalization of p* LUMO and p HOMO of the intercalation compounds over I.

Key words [QUANTUM CHEMISTRY](#) [CNDO APPROXIMATION](#) [CONJUGATED DOUBLE BOND COMPOUNDS](#) [LITHIUM](#) [ELECTROCHEMISTRY](#) [POLYPYRROLE](#) [FRONTIER ORBITAL THEORY](#) [EMBEDDING COLLISIONS](#)

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