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长链烷烃分子吸附增强效应的**STM**图像理论研究

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摘要 STM实验发现长链烷烃分子能够改善多种有机分子的吸附性能，
本文利用CVFF力场对长链烷烃与石墨吸附体系进行了分子力学模拟，用半经验ZINDO/1，AM1
方法对烷基取代酞菁和卟啉的STM形貌反差机制进行了研究。理论计算表明，
长链烷烃分子与基底的吸附作用增强了分子的吸附稳定性，
而烷烃分子间的二维结晶作用使取代酞菁和卟啉分子形成密排的二维有序结构。前线轨道电子密度和STM实验结果比较证明，
分子核部分的电子性质和烷基部分的几何结构决定了取代酞菁和卟啉分子的STM形貌反差。

关键词 烷烃 卟啉 酞菁P 二维结构

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Theoretical study of adsorption effects of long chain alkane system in STM images

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Abstract STM observation shows that long chain alkanes increase the adsorption stability of organic molecules. In this work, the interactions of long chain alkanes adsorbed on graphite surface were simulated by molecular mechanics and the STM imaging mechanism of alkylated phthalocyanine and porphyrin was studied by semiempirical quantum mechanics method of ZINDO/1 and AM1. The calculated results illustrated that the interactions between adsorbed molecule and substrate enhanced the stability and immobility of adsorbate, and the interactions between adsorbed molecules determined the form of two- dimensional structure. Compared the electron density contour of the frontier molecular orbits, it was indicated that the STM image contrast of alkylated Copper (Ⅱ) phthalocyanine and porphyrin was attributed to the electronic effects of the core of phthalocyanine and porphyrin and topographic effects of alkyl.

Key words ALKANE PORPHYRIN ZINC PHTHALOCYANINE

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