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TiO_2纳米膜上吸附态甲基橙的光催化降解反应活性研究

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摘要 以反胶束溶液不同陈化是间及涂膜次数制备了三种TiO_2纳米膜，用XRD，SEM和AFM方法考察了这些膜的形态结构特征，以吸附态甲基橙为模型反应物，研究 TiO_2纳米膜的光催化降解活性，并以AM1分子模拟计算探讨了甲基橙分子在不同膜 上可能的吸附态，及其与光催化降解的关联。结果表明，膜A最薄，膜上纳米粒子 分布均匀，表面平滑，甲基橙分子可能主要以端基方式吸附，这种吸附对分子骨架 化学键的影响较小，且不利于表面羟基对底物分子的进攻，结果反应活性低。膜B 最厚，对光的透过率最低，膜上纳米粒子分布很不均匀，表面缺陷结构丰富，对甲 基橙的吸附强，甲基橙分子主要以平卧式吸附，从而削弱了分子中的N=N双键，有 利于表面痉基对底物分子的进攻，光催化反应活性最高。膜C的厚度和粒子分布的 均匀性介于膜A和膜B之间，甲基橙分子可以两种方式吸附光催化反应的活性介于膜 A和膜B之间。

关键词 二氧化钛 纳米相材料 甲基橙 光催化 降解 催化活性

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Study of Photocatalytic Degradation Activity of Methyl Orange Adsorbed on TiO_2 Nano-Films

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Abstract TiO_2 nano-films have been prepared by dip coating in a reverse micelle solution at different periods of gelation. The morphologic and structural characteristics were examined by using XRD, SEM and AFM methods. Photocatalytic reduction of the dye methyl orange adsorbed on the TiO_2 nano-films was also studied. Molecular AM1 modeling calculation was carried out for understanding the behavior of the dye adsorption and decomposition on the films. The film made at an early state of gelation is thinnest and uniform in the distribution of nano- particles on the film. The methyl orange molecule may be adsorbed on the film only by the oxygen atom of the sulfonate group through electronic force and coordination from the oxygen atom to the surface of the film. Such a terminal group adsorption has little effect on the bond structure of the whole molecule and may not be benefit to the attacking of surface hydroxyl onto the reactant, resulting in low photocatalytic activity. The film made by repeating coating ten times in the early state of gelation shows high roughness due to the large aggregates formed by the interconnected TiO_2 nano-particles, and crackings can also be observed. But the film possesses a high capacity of adsorption and high photocatalytic activity for the dye. The methyl orange molecule may lie on the surface of the film in feedback coordination from surface hydroxyl to the conjugated π bond, besides the terminal group coordination, since the film possesses large defect and thus high density of active sites. Such an adsorption not only weakens the large conjugated π bond structure throughout the whole molecule but also favors the attacking of surface hydroxyl onto the adsorbed molecules. The film made at 6 hours of gelation by dip coating once shows higher roughness and the surface particles are of bigger agglomerates. The capacity and photoreactivity of the film are moderate since its defect and active density are also moderate.

Key words TITANIUM DIOXIDE NANOPHASE MATERIALS METHYL ORANGE PHOTOCATALYSIS DEGRADATION CATALYTIC ACTIVITY

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