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TiO2纳米晶电极上半菁衍生物分子设计中空间位阻效应的研究

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摘要 设计合成了具有不同空间位阻的吡啶盐类和喹啉盐类半菁染料(E)-N-(4—磺酸 根丙基)-4-[2-4（4-N，N-二乙基氨基苯基）乙烯基]吡啶鎓盐（EPS），（E）-N-(4- 磺酸根丁基）-4-[2-(4-N,N-二乙氨基苯基）乙烯基]吡啶鎓盐（EPS4）和（E） -N-（4-磺酸根丁基）-4-[2-（4-N，N-二乙基氨基苯基）喹啉鎓盐（EQS4），研究了它们 的光物理性质，并将它们用作TiO2纳米晶电极的光敏化剂引入光电化学电池中。 研究发现: 对于吡啶类半菁染料而言，无论是以三个亚甲基或是以四个亚甲基来连接 吸附基团RSO3^-和发色团时，单个的EPS和EPS4分子的光电响应行为一致．但是由于 以三个亚甲基来连接时，与EPS4相比，染料EPS的空间位阻相对较小，有利于其在 多孔膜上的吸附，最终结果是染料EPS对TiO2纳米晶电极的敏化作用好于EPS4．以喹啉 环为受电子基团的染料EQS4与同样含有四个亚甲基的以吡啶环为受电 子基团的EPS4相比，单个EQS4分子的光电响应行为虽然好于EPS4分子，但由于 EQS4分子间的空间位阻较大，影响了它在多孔电极上的吸附，致使其敏化的太阳能电池的总光电转换效率有所下降.

关键词 二氧化钛 纳米相材料 电极 半菁 吡啶 P 喹啉 P 太阳能电池

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Steric Hindrance Effect of Hemicyanine Derivatives on Their Spectral Sensitization Efficiencies of Nanocrystalline TiO_2 Electrodes

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Abstract Three novel hemicyanine derivatives, (E)-N-(4-sulfopropyl)-4-[2-(4- N, N-diethylaminophenyl)-ethenyl] pyridinium (EPS), (E)-N-(4-suMbbutyl)- 4-[2-(4-N, N-diethylaminophenyl)ethenyl]pyridinium (EPS4), and (E)-N-(4-su)fobutyl)-4-[2-(4-N, N-diethylaminophenyl)ethenyl]quinolinium (EQS4) with different length of alkyl chains between the adsorbing group (RSO3-) and the chromophore group, were synthesized and their photophysical and photoelectrochemical properties were studied. Experimental results show that using either three-methylene group or four-methylene group to link the adsorbing group and the chromophore group has little effect on the photoelectrical response of dye, but this difference has great impact on the adsorbance properties of dye on nanocrystalline electrode. EPS, bearing a chain of three-methylene group, has a greater adsorbed molecule amount on nanocrystalline TiO2 film because of small steric hindrance effect compared with EPS4. So EPS-sensitized solar cell generated a higher overall photon to electric conversion efficiency. Compared with EPS4, the photoelectrical response of dye EQS4 was greatly improved when a stronger electron acceptor was introduced. However, samely due to the steric hindrance effect, the adsorption number of EQS4 on mesoporous TiO2 film (2.99 * 1016 molecules ? cm-2) dropped down drastically compared with that of EPS4 (6.26 * 1016), and at last EQS4-sensitized solar cell generated a lower overall photoelectrical conversion yield compared with EPS4.

Key words TITANIUM DIOXIDE NANOPHASE MATERIALS ELECTRODE hemicyanine PYRIDINE P QUINOLINE P SOLAR CELLS

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