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The Study of Adsorption of RuP onto TiO₂ (110) Surface Using Photoemission Deposited by Electrospray

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Abstract: Countries worldwide rely on electric power as a critical economic growth and progress factor. Renewable energy sources, often referred to as alternative energy sources, such as wind, solar energy, geothermal energy, biomass, and hydropower, have garnered significant interest in response to the rising consumption of fossil fuels. Dye-sensitized solar cells (DSSCs) are a highly promising alternative for energy production as they possess numerous advantages compared to traditional silicon solar cells and thin-film solar cells. These include their low cost, high flexibility, straightforward preparation methodology, ease of production, low toxicity, different colors, semi-transparent quality, and high power conversion efficiency. A solar cell, also known as a photovoltaic cell, is a device that converts the energy of light from the sun into electrical energy through the photovoltaic effect. The Gratzel cell is the initial dye-sensitized solar cell made from colloidal titanium dioxide. The operational mechanism of DSSCs relies on various key elements, such as a layer composed of wide band gap semiconducting oxide materials (e.g. titanium dioxide $[TiO_2]$), as well as a photosensitizer or dye that absorbs sunlight to inject electrons into the conduction band, the electrolyte utilizes the triiodide/iodide redox pair $(I - /I_3 -)$ to regenerate dye molecules and a counter electrode made of carbon or platinum facilitates the movement of electrons across the circuit. Electrospray deposition permits the deposition of fragile, non-volatile molecules in a vacuum environment, including dye sensitizers, complex molecules, nanoparticles, and biomolecules. Surface science techniques, particularly X-ray photoelectron spectroscopy, are employed to examine dye-sensitized solar cells. This study investigates the possible application of electrospray deposition to build highquality layers in situ in a vacuum. Two distinct categories of dyes can be employed as sensitizers in DSSCs: organometallic semiconductor sensitizers and purely organic dyes. Most organometallic dyes, including Ru533, RuC, and RuP, contain a ruthenium atom, which is a rare element. This ruthenium atom enhances the efficiency of dye-sensitized solar cells (DSSCs). These dyes are characterized by their high cost and typically appear as dark purple powders. On the other hand, organic dyes, such as SQ2, RK1, D5, SC4, and R6, exhibit reduced efficacy due to the lack of a ruthenium atom. These dyes appear in green, red, orange, and blue powder-colored. This study will specifically concentrate on metal-organic dyes. The adsorption of dye molecules onto the rutile TiO2 (110) surface has been deposited in situ under ultra-high vacuum conditions by combining an electrospray deposition method with X-ray photoelectron spectroscopy. The X-ray photoelectron spectroscopy (XPS) technique examines chemical bonds and interactions between molecules and TiO₂ surfaces. The dyes were deposited at varying times, from 5 minutes to 40 minutes, to achieve distinct layers of coverage categorized as sub-monolayer, monolayer, few layers, or multilayer. Based on the O 1s photoelectron spectra data, it can be observed that the monolayer establishes a strong chemical bond with the Ti atoms of the oxide substrate by deprotonating the carboxylic acid groups through 2M-bidentate bridging anchors. The C 1s and N 1s photoelectron spectra indicate that the molecule remains intact at the surface. This can be due to the existence of all functional groups and a ruthenium atom, where the binding energy of Ru 3d is consistent with Ru2+.

Keywords: deposit, dye, electrospray, TiO2, XPS

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