

Resolving the molecule-oxide interface of dye-sensitized solar cells at the atomic level

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Dye-sensitized solar cells (DSSCs) constitute a promising approach to sustainable and low-cost solar energy conversion. The modification of TiO₂ anatase surfaces with organic and organometallic molecules is essential to high DSSC conversion efficiencies which crucially depend on the effective coupling of photosensitizers to the substrate. Despite the widespread use of TiO₂ anatase surfaces, however, there has been little work investigating the structural and electronic properties of adsorbed dye molecules at the single molecule level. We report on a combined experimental and theoretical study of the geometric and electronic properties of the photosensitizer N3 (cis-bis(isothiocyanato)bis(2,2'-bipyridyl-4,4'-dicarboxylato)-ruthenium(II)) adsorbed on TiO₂ anatase (101). In situ electrospray ionization deposition combined with scanning tunnelling microscopy and spectroscopy studies in ultra high vacuum at low temperature provide direct access to the dye-substrate interface at the atomic level. Our experiments probe the local electronic structure with single molecule sensitivity revealing multi-conformational N3 binding geometries on the oxide support as well as mutual interactions between dye molecules. The spectroscopic characterization demonstrates the existence of ideal dye adsorption configurations for maximum charge injection efficiencies.