

Investigating Relative Binding Strengths of Various Dye Attachment Chemistries at the Titania-Dye Interface in Dye-Sensitized Solar Cells

G. J. Smith,^{1,+} B. Harvey,², J. Placzek³

¹ Department of Chemistry & Biochemistry, Angelo State University, San Angelo, TX, USA

² Department of Chemistry & Biochemistry (Undergraduate), Angelo State University, San Angelo, TX, USA.

³ Department of Chemistry & Biochemistry (Undergraduate), Angelo State University, San Angelo, TX, USA.

Dye-sensitized solar cells (DSSC) continue to be a promising area of research in our society's quest for clean and renewable energy. Typically, in these solar cells light is harvested by a dye molecule which is covalently bound to a mesoporous semiconducting material, most commonly titania. The excited electron is injected into the semiconductor and moves down to the electrode. One of the most important parts of these solar cells is the interface between the dye and the semiconductor. Optimally, the bond between dye and semiconductor should be strong, yet allow for rapid electron transport from excited dye to semiconductor. The most common chemistry for this attachment is with one or more carboxylate groups. There is a surprising lack of information about the performance of other chemistries in the literature, particularly experimental evidence. Some theoretical calculations have been performed¹, but it would be very useful to have a library of the experimental performance of various attachment chemistries that could be used when considering specific dyes or in the synthesis of new dye molecules.

Here, we discuss a systematic method to compare the strength of the attachment of different chemistries to titania surfaces. To be able to directly compare chemistries, a model set of molecules were used, each 18 carbons in length capped with the group being studied. These molecules were used to form a self-assembled monolayer on a flat titania surface, then exposed to a typical solvent used in DSSCs at a slightly elevated temperature for 24 hours. The quality of the monolayer was measured before and after exposure using goniometry and ellipsometry. Table 1 shows the amount of degradation seen in each group studied. A description of the method, a comparison of the results, and how the results compare to previous theoretical studies will be included in discussion.

Terminal group:	Carboxyl	Thiol	Silane	Phosphonic acid
Degradation:	15.7 %	53.9 %	33.2 %	38.1 %

Table 1. Degradation of each monolayer after exposure to ethanol at 30°C for 24 hours.

[1] F. Ambrosio, N. Martsinovich, A. Troisi, J. Phys. Chem. Lett. **3**, (2012).

⁺Author for correspondence: Gregory.Smith@angelo.edu