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Atomic Layer Deposition of TiO2 on Transparent Conductive Oxide Nanoparticles for Solar Energy Conversion

The deposition of TiO2 thin films onto transparent conducting oxide (TCO) surfaces is of immense interest to a broad range of solar energy conversion applications. For example, TiO2 has been recently used as a buffer layer in photovoltaic (PV) applications as well as a photoactive layer or protective layer in photoelectrochemical (PEC) and photocatalytic applications. Furthermore, since many of these applications seek to deposit this layer onto porous scaffolds with angstrom-level thickness precision, atomic layer deposition (ALD) is seen as an essential tool to achieve such high precision control without sacrificing conformality and uniformity. In this presentation, we will cover two studies where we have explored some of the unique properties of using TiO2 films grown by ALD.

In the first study, we analyze the water-oxidizing PEC performance of TiO2 photoanodes synthesized by ALD of TiO2 onto a porous, transparent, and conductive fluorine-doped tin oxide nanoparticle (nanoFTO) scaffold. Our results show how coupling the nanoFTO nanostructure with ultrathin conformal ALD TiO2 coatings offers advantages including the orthogonalization of charge transport/transfer with absorption, complimentary photon adsorption, and favorable interfaces for charge separation and transport. The fundamental mechanisms behind the advances are characterized via a variety of electrochemical techniques and contrasted with those of pure single crystal rutile TiO2 NWs. The strategies from this work highlight the opportunities inherent to heteronanostructures with thin films deposited by ALD and may be applied to improve the PEC conversion efficiencies of other promising materials whose absorption properties are more compatible with the AM 1.5G spectrum.

In a more recent second study, we have examined how the use of different deposition temperatures during TiCl4/H2O-based ALD TiO2 growth can drastically alter the interface between TiO2 and three common TCO materials, namely: indium tin oxide (ITO), fluorine-doped tin oxide (FTO), and antimony-doped tin oxide (ATO). Additionally, by conducting the ALD on high surface area TCO nanoparticles, we amplified the effects of the surface reactions, which enabled us to visually detect a drastic change in color after just 3 ALD cycles at a given temperature. A deep examination of their photoelectron spectra yields insights into the surface reactions that occur under these ALD conditions. Moreover, we find that the modification of this buried TiO2/TCO interface can profoundly impact the final device's energy conversion efficiencies and thus warrants a deeper understanding.