Understanding Surface Chemistry of Atomic Layer Deposition: Toward Renewable Energy Applications

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With the intensifying interest in functional nanoscale materials for applications in electronics and energy conversion, methods for fabricating materials with atomic-level control are becoming increasingly important. Atomic layer deposition (ALD) is a method that provides excellent capabilities for depositing thin films, nanoparticles, and other nanoscale materials. This talk will describe research into the surface chemistry occurring during ALD, focusing on the ALD of metal oxides of interest for renewable energy applications. Deposition of binary, ternary, and doped metal oxides at a range of important interfaces has already been demonstrated using ALD. However, a fundamental understanding of the growth process for metal oxides is still lacking. Moreover, it is often difficult to correlate the material properties and growth characteristics with the process parameters due to the limited understanding of the underlying surface chemistry. In this talk, we will describe the results of both *in situ* and *ex situ* studies investigating nucleation in metal oxide deposition, using zinc tin oxide (ZTO) as a model system. Based on a combination of quadrupole mass spectrometry, infrared spectroscopy, low energy ion scattering, and density functional theory, we propose mechanisms explaining the presence of a nucleation delay that occurs when the metal oxide processes are mixed. The application of ALD metal oxides to renewable energy applications will also be presented. We will examine both a photovoltaics application, in which ALD is used to deposit layers in thin film solar cells, and an application in clean fuel synthesis for which ALD produces active electrocatalysts.

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