A toolbox for an all-ALD earth-abundant resonant tunneling junction solar cell

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Atomic layer deposition (ALD) enables the fabrication of high-quality electronic materials and interfaces through the careful design of chemical precursors and control of process conditions.The fabrication of third-generation, scalable photovoltaic devices requires a toolbox of high-performance, safe, and facile processes for the deposition of functional materials using only earth-abundant elements. Such a suite of processes does not readily exist, so we began exploring each stage of the development cycle of a device from precursor design, process development, device simulation, to fabrication. Here are some new ALD options.

F-doped SnO_2 (FTO) and lead sulfide (PbS) are promising earth-abundant candidates for transparent conducting oxide (TCO) top contacts and tunable semiconducting photo-absorbers, respectively.We have prepared divalent homoleptic precursors from inexpensive and readily available reagentsthat display exceptional thermal stability and volatility: tin(II) bis(trifluoroacetate) (1 Torr/170 °C, dec.425°C) and N^2,N^3-di-tert-butylbutane-2,3-diamido lead(II) (1 Torr/92 °C, dec.150 °C). In addition, we have circumvented typical hazards associated with fluorinated and sulfide ALD processes by eliminating HF from our FTO process with a single-source fluorinated precursor, and H_2S from our PbS processwith tert-butylthiol.

Together theseenable the combination of two promising strategies to exceed the efficiency limits of traditional photovoltaics:energy-selective contacts and multiple quantum well (MQW) resonant tunneling junctions. ALD of everylayer gives sub-nanometer thickness control simply by changing the number of cycles performed thus allowing unprecedented design freedom. To aid in the design of a final device, we solved the 1D Schrodinger-Poisson equation to simulate the resonant tunneling currentthrough multiple Al_2O_3/PbS/Al_2O_3 wells in our architecture.This presentation will cover the challenges associated with developing safe ALD precursors for high-performance electronics, the behaviour and quality of the resultant films, and give an outlook on the possible performance of an all-ALD resonant tunnel junction solar cell.