

Abstract Submitted
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High photoactivity in ultrathin as-grown hematite films prepared by atomic layer deposition¹ JEFFREY KLUG, NICHOLAS BECKER, SHANNON RIHA, ALEX MARTINSON, JEFFREY ELAM, MICHAEL PELLIN, THOMAS PROSLIER, Argonne National Laboratory — Nanostructured hematite (α -Fe₂O₃) has been widely studied for use in a variety of thin film applications including solar energy conversion, water oxidation, catalysis, and gas sensing. Among established deposition methods, atomic layer deposition (ALD) is a leading technique for large-scale, controlled synthesis of a wide range of nanostructured materials. In this work, ALD of Fe₂O₃ is demonstrated using FeCl₃ and H₂O precursors at growth temperatures between 200 – 350°C. Self-limiting growth of Fe₂O₃ is observed with a growth rate of ~ 0.06 nm/cycle. As-deposited, films are nanocrystalline with low Cl impurities and a mixture of α - and γ -Fe₂O₃. Post-deposition annealing in O₂ leads to phase-pure hematite with increased out-of-plane grain size. Photoelectrochemical measurements under simulated solar illumination reveal high photoactivity toward water oxidation in both as-deposited and post-annealed films. Planar films deposited at low temperature (235°C) exhibit remarkably high photocurrent densities ~ 0.71 mA/cm² at 1.53 V vs. the reversible hydrogen electrode (RHE) without further processing. Films annealed in air at 500°C show current densities of up to 0.84 mA/cm² (1.53V vs. RHE).

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