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Single-source precursors for \( \alpha \)-Fe\(_2\)O\(_3\) thin-films

Matthew K. Surman\(^{a,b}\), Michael. S. Hill\(^b\) and Andrew L. Johnson\(^b\)

\(^a\) Centre for Doctoral Training in Sustainable Chemical Technologies, University of Bath, BA2 7AY.
\(^b\) Department of Chemistry, University of Bath, BA2 7AY.

E-mail: mks48@bath.ac.uk URL: http://www.bath.ac.uk/csct

Introduction

Photoelectrochemical water-splitting is one method of producing hydrogen from non-hydrocarbon primary energy sources. Photoelectrochemical water-splitting is often performed using metal oxide thin-films\(^1\), which ideally will have:

- A band-gap of sufficient energy for efficient absorption of the solar spectrum
- A band-gap whose valence and conduction band energies bridge the redox potentials of the two relevant half-reactions:

\[
\begin{align*}
4\text{H}^+ + 4\text{e}^- &\rightleftharpoons 2\text{H}_2, & E_{\text{redox}} &= 0.0 \text{ V} \\
\text{O}_2 + 4\text{H}^+ + 4\text{e}^- &\rightleftharpoons 2\text{H}_2\text{O}, & E_{\text{redox}} &= 1.23 \text{ V} \\
2\text{H}_2\text{O} &\rightarrow 2\text{H}_2 + \text{O}_2, & E_{\text{redox}} &= -1.23 \text{ V}
\end{align*}
\]

Deposition of \( \alpha \)-Fe\(_2\)O\(_3\) thin-films

- \( \alpha \)-Fe\(_2\)O\(_3\) has a band-gap of 1.9-2.2 eV, making it a suitable photo absorber for water-splitting\(^2\).
- Iron is earth-abundant and cheap, making hematite an inherently sustainable material.
- AA-CVD can be used to deposit a wide selection of single-source precursors.\(^3\)

Precursor design

- The iron complex Fe(hfa)\(_2\))TMEDA has been shown to be a useful precursor for the deposition of \( \alpha \)-Fe\(_2\)O\(_3\).\(^4\)
- At elevated temperatures the TMEDA ligand is labile, making the precursor involatile.
- By modifying the (fac) ligands to bear a pendant donor group we may be able to increase the stability of precursors.

Future work

- A second series of mono-substituted iron (II) complexes will be synthesised using the ketoiminate ligands we have developed.
- Synthesised hematite precursors will be analysed using thermogravimetric analysis.
- Based on the decomposition observed by thermogravimetric analysis, lead precursors will be chosen for deposition by AA-CVD.
- Hematite-thin films will be produced and fully characterised.
- Devices will be manufactured and tested for photoelectrochemical water-splitting.

Conclusions

- A series of ketooiminate ligands and their sodium complexes have been synthesised and fully characterised.
- From the sodium salts, a series of potential single-source precursors for hematite have been synthesised and fully characterised.

References


\[\text{Fe}[\text{NaL}_2]\text{O}_2\text{Fe}[\text{NaL}_2] \]