Monolithically Integrated Thin-Film/Si Tandem Photoelectrodes

Author Name: Zetian Mi
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MONOLITHICALLY INTEGRATED THIN-FILM/SILICON TANDEM PHOTOELECTRODES FOR HIGH EFFICIENCY AND STABLE PHOTOELECTROCHEMICAL WATER SPLITTING

Zetian Mi, University of Michigan, Ann Arbor
Thomas Hamann, Michigan State University
Dunwei Wang, Boston College
Yanfa Yan, University of Toledo

Project Vision

We propose to develop monolithically integrated thin-film/Si tandem photoelectrodes to achieve both high efficiency (>15%) and stable (>1,000 hrs) water splitting systems.

Project Impact

Success of the project will help meet the DOE 2020 target (20% solar-to-hydrogen efficiency and $5.70 per kg H₂) and pave the way for widespread commercialization of solar hydrogen production technologies.
Innovation and Objectives

Project history
The applicants have had complementary expertise in PEC water splitting:
- $\text{Ta}_3\text{N}_5$, BCTSSe, and InGaN top photoelectrodes with $E_{\text{g}} \sim 1.7-2$ eV.
- Low resistivity nanowire tunnel junction on Si wafer.
- Ultrathin N-rich GaN coating against photocorrosion and oxidation.

Proposed targets

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<tr>
<th>Metric</th>
<th>State of the Art</th>
<th>Proposed</th>
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<td>STH Efficiency / Stability</td>
<td>16% 1.5 hrs</td>
<td>&gt; 15% 1000 hrs</td>
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Barriers
- Further improve the performance and stability of top photoelectrodes.
- Integration of the top photoelectrodes with the Si bottom light absorber through nanowire tunnel junction.

Partnerships
- **Thomas Hamann, Michigan State Univ.**:
  Ta$_3$N$_5$, PEC characterization
- **Dunwei Wang, Boston College**:
  Cocatalyst deposition, surface protection
- **Yanfa Yan, Univ. Toledo**:
  Sputtering deposition and PEC characterization of BCTSSe
Technology Innovation

- The use of Si substrate as the bottom light absorber to reduce the cost of PEC water splitting.
- The use of recently developed low cost \( \text{Ta}_3\text{N}_5 \), BCTSSe, and \( \text{In}_{0.5}\text{Ga}_{0.5}\text{N} \) photoelectrodes as the top light absorber, which have a direct energy bandgap of 1.7-2.0 eV.

\( \text{Hu}, \text{S. et al.}, \text{Energy Environ. Sci.}, 6 (2013), 2984–2993. \)
Ill-nitrides are the only known semiconductors whose energy band edges can straddle water redox potentials under deep visible and near-IR light.

N-terminated surface protecting against corrosion and oxidation

- Ga polarity
  - Unstable
  - Difficult to extract holes

- N polarity
  - Stable
  - Efficient hole extraction
InGaN nanowires with various sizes and surface morphology can be grown, with energy bandgap tuned from the visible to the infrared.

The N-terminated surfaces of InGaN nanowires protect against photocorrosion and oxidation, leading to long-term stable operation in overall water splitting.

*Nature Commun.*, vol. 6, 6797, 2015.
We will also develop both BCTSSe and Ta₃N₅ thin films as efficient photocathodes and photoanodes for PEC water splitting.
Nanowire tunnel junction will be used to connect to the top light absorber (Ta₃N₅, BCTSSe, or InGaN) with the Si bottom junction.

The use of nanowire tunnel junction can further reduce the formation of defects and dislocations in the top light absorber.

*Nano Letters*, vol. 15, 2721, 2016.
Effective Leveraging of the EMN Resource Nodes

- **Glenn Teeter, NREL:** Surface analysis cluster tool, surface measurements
- **Francesca Toma, LBNL:** Photoelectrochemical AFM and STM
- **Todd Deutsch, NREL:** Surface modifications and protection
- **Tadashi Ogitsu, LLNL:** Ab initio modeling of electrochemical interfaces
Thank you!