Materials for Energy. Theoretical Challenges and ...

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"Energy can be neither created nor destroyed, but can only be transformed from one form to another"
Case studies (subset)

- Energy and materials - a continual and mutually enriching relationship
- Materials used to produce / transform / store energy for our necessities
- Energy allows production of a broad range of materials for society

Case studies (where theory helps)

Production
- Energy from HEAT: Water to hydrogen from nuclear or solar heat
- Energy from LIGHT: Photovoltaic cells

Consumption
- Energy Transformation: Hydrogen to Electricity + Water (Fuel cells)
- Energy-Saving Materials: Lubrication, insulation, illumination
**Water to hydrogen problem (through heat)**

### NUCLEAR

- Berm
- Intermediate Loop Circulator
- Modular Helium Reactor
- Intermediate Heat Exchanger
- Primary Coolant Circulator
- Electricity
- Low fuel cost
- High T burns actinides
- Use waste heat

### SOLAR

![Solar Power Plant](image)

- **Compatible with 7.5$/gallon gasoline**
- **Materials** [problems: catalysis, corrosion, hydrogen embrittlement (nano-technology, coatings, alloys)]

### Table: Comparison of Processes

<table>
<thead>
<tr>
<th>Process</th>
<th>Nuclear S-I</th>
<th>Solar S-I</th>
<th>Solar Hi T S-I</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature °C</td>
<td>900</td>
<td>900</td>
<td>1100</td>
</tr>
<tr>
<td>Efficiency - Heat to H₂</td>
<td>52%</td>
<td>52%</td>
<td>56%</td>
</tr>
<tr>
<td>Hydrogen cost, $/kg*</td>
<td>1.42</td>
<td>3.45</td>
<td>2.50 **</td>
</tr>
</tbody>
</table>

*Including a 0.20$/Kg for O₂ premium*
**Conversion example**

**Sulfur Iodine Cycle**

GOOD for NuH₂, SolarH₂

**Catalyst:** Pt, Cu, Fe₂O₃, efficiency, size, nucleation, sintering..

**Coolants:** Molten Salts, Lead, Lead-Bismuth..

**Corrosion:** Si-rich steel, SiC, Si₃N₄, coatings, Pt, Au, ceramics...

**nano-catalysis is not** nano+catalysis

"size-induced nucleation of inactive phases (size pressure approximation)"

**PRL 100, 195502 (2008)**

**PRB, 78, 054105 (2008)**
STRUCTURE PREDICTION PROBLEM

“One of the continuing scandals in the physical sciences is that it remains in general impossible to predict the structure of even the simplest crystalline solids from a knowledge of their chemical composition….”

[John Maddox, Nature 1988, (editor 22 years)]
.. the problem is even worse... nano-thermodynamics
Photovoltaics: challenges

- I PVs: based on crystalline Si $pn$ junctions – medium high efficiency (25%)
- II PVs: multi-junctions – high efficiency (35 %) [42.7%, U. Delaware with concentrators]
- IIIa PVs: novel approaches using “exotic concepts (hot carriers, multi-e-h pairs, thermophotonics – high cost - high efficiency - still in infancy
- IIIb: Organics – low efficiency but very low cost: good optical absorption coefficients, plastic compatible, easy fabrication

*(Shaheen, MRS Bulletin, (2005))*
A theoretical nightmare

Efficiency

\[(1-R) \eta_A \eta_{ED} \eta_{CT} \eta_{CC}\]
Hydrogen consumption!
Fuel cells: catalysis + diffusion

- Basic operation of a fuel cell.
- The net input of the fuel cell is hydrogen and oxygen.
- Its net output is water, electricity, and heat.
- Some heat is required to start the process (not too much but not too little).

\[
\begin{align*}
H_2 & \rightarrow 2H^+ + 2e^- \\
\text{hydrogen oxidation} \\
4H^+ + 4e^- + O_2 & \rightarrow 2H_2O \\
\text{oxygen reduction}
\end{align*}
\]
Energy-saving challenge: superlubrication

Study of commensurability between interfaces with and without contaminants

Adsorbed CH$_4$ on d-AlNiCo

Ordering of Methane on AlNiCo surface

commensurability ↔ high friction

Hirano, et al, PRB 41, 11837 (1990)
Da Vinci (original)
The scientific challenge of our century

Energy production, transformation, storage, consumption, and disposal are challenges for

- materials scientists
- condensed-matter physicists
- engineers
- mathematicians

exciting challenges for our

Center for Theoretical and Mathematical Sciences

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