Sustainable Chemistry in the CAS Databases

247th ACS National Meeting & Exposition
It’s not easy being green...
Agenda

- Green Chemistry Techniques
- New Energy Storage Materials
- More Efficient Biomass Conversion
- Advanced Methods for Water Purification
- Q & A
Green Chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous materials in the design, manufacture and application of chemical products.
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Green chemistry articles appear in every scientific area covered in the CAS Databases

- Over 26,000 references
- ~3,400 related patents from the 63 patent authorities covered in CAS databases
- Thousands of reactions and structures involving green chemistry
Pharma companies, chemical manufacturers, silicon chip producers, etc., are increasingly turning to green chemistry in an effort to reduce waste, costs and develop environmentally benign processes

- **Green Catalysis**
  - Biocatalysis
  - Organocatalysis
  - Supported catalysis
  - Fluorous catalysis
  - Catalytic direct C-H bond activation reactions

- **Green Synthetic Techniques**
  - Alternative solvents
  - Atom economic multi-component reactions
  - Microwave and ultrasonic reactions
  - Solid-supported synthesis
  - Fluorous and ionic liquid-based recycling techniques
  - Flow reactors
Chemoenzymatic drug synthesis has become popular in recent years, due to growing demand for “greener” and more cost-effective processes.

- Benefits of biocatalysis over chemical synthesis:
  - Aqueous solutions
  - Room temp. and atmospheric pressure
  - Highly selective
  - Enzymes can be re-used for many cycles
  - High yields
  - Economically efficient

- Enzymes can be broadly categorized in six major classes:
  - Hydrolases (hydrolysis reactions in water)
  - Oxidoreductases (oxidation or reduction)
  - Transferases (transfer of a group from one molecule to another)
  - Lyases (non-hydrolytic bond cleavage)
  - Isomerases (intra-molecular rearrangement)
  - Ligases (bond formation requiring triphosphate)
Let’s find “green” techniques to synthesize Atorvastatin, a cholesterol-lowering statin
We found various “green” synthetic pathways catalyzed by hydrolases and proteases.
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Nanotechnology is the key to new energy storage breakthroughs

- Nanomaterial Technologies
  - Organic and printed electronics
  - Nano-coatings
  - Nano-composites
  - Nano-fluids
  - Nano-catalysts
  - Nano-carbons
  - Nano-electrodes

- Real life applications
  - Cheaper, more efficient solar cells
  - Extended battery storage capacity (batteries for electric cars and lithium-ion batteries)
Nanopillars are novel nanostructures that trap more light and could lead to cheaper solar cells.
Full-text U.S. patents are readily available with only one click, without the need to navigate to an external website.

**Coming soon**
- EPO
- WIPO
- Germany
- France
- U.K.
- Russia

### United States Patent Application Publication

<table>
<thead>
<tr>
<th>Inventors</th>
<th>Mark D. Hall, Austin, TX (US), Mehul D. Shroff, Austin, TX (US)</th>
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</thead>
<tbody>
<tr>
<td>Assignee</td>
<td>FREESCALE SEMICONDUCTOR, INC., Austin, TX (US)</td>
</tr>
<tr>
<td>Appl. No.</td>
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<tr>
<td>Filed</td>
<td>Jun. 29, 2012</td>
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</tbody>
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**Abstract**

A disclosed method of fabricating a hybrid nanopillar device includes forming a mask on a substrate and a layer of nanoclusters on the hard mask. The hard mask is then etched to transfer a pattern formed by the first layer of nanoclusters into a first region of the hard mask. A second nanocluster layer is formed on the substrate. A second region of the hard mask overlying a second region of the substrate is etched to create a second pattern in the hard mask. The substrate is then etched through the hard mask to form a first set of nanopillars in the first region of the substrate and a second set of nanopillars in the second region of the substrate. By varying the nanocluster deposition steps between the first and second layers of nanoclusters, the first and second sets of nanopillars will exhibit different characteristics.

![Diagram showing bonded layer and nanopillar structure]
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Interest from first-generation biofuels has shifted to cellulosic ethanol, biobutanol and algae-based biofuels

- Biomass feedstock can be converted into cellulosic ethanol via enzymatic breakdown, a process already in widespread commercial use
  - Biomass feedstock $\rightarrow$ Cellulose $\rightarrow$ Sugars $\rightarrow$ Cellulosic Ethanol
  - Cellulose conversion can be improved by ~ 50% via pretreatment

- Recent discovery shows that cellulosic ethanol can be converted into butanol, a more attractive alternative to ethanol
  - Biobutanol has high energy content
  - Compatible with existing vehicles and fueling infrastructure

- Conversion of algae to biofuels is another area of high R&D interest
  - Algae contain more biofuel lipid precursors per unit area
  - Grow faster, and can be harvested quicker
BP Biofuels has reported an innovative way of making biobutanol using ruthenium phosphine catalysts

- Technology can be applied not only to petrochemical sources, but to biological sources as well
  - High selectivity
  - High conversion rates (> 20%)
  - Can be used to convert cellulosic ethanol to butanol
Recent patent shows a new method of extracting biofuel lipid precursors from algae

- Cost effective, economically viable method to create biofuels
  - Uses a hydrolysis reactor
  - No thermal separation
  - No dewatering and drying
  - No extraction of immobilized lipids
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Water purification methods date back to 1800s, but current approaches are very sophisticated

- Basic water purification methods
  - Boiling
  - Chlorine treatments
  - Distillation
  - UV light
  - Ceramic filters

- Advanced water purification methods
  - Reverse osmosis
  - Micro & Ultrafiltration
  - Nanofiltration
  - Subnanoscale filtration
MIT has recently devised a method to create atomically thin graphene filters with subnanoscale pores

- Advantages over nanofiltration & reverse osmosis
  - High permeability (> 50 times larger than conventional membranes)
  - Controllable pore size (may allow water, but filter everything else)
  - Suitable for biological applications (i.e., removal of unreacted agents from DNA)

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