Distributed Research: A New Paradigm for Undergraduate Research and Global Problem Solving

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There is no question that identifying and developing new renewable energy sources is a top priority for mankind. Solar energy is the only available source of energy capable of continually providing the immense amounts of carbon-free energy necessary to keep CO_2 levels in the atmosphere below dangerous levels. Photoelectrolysis of water with sunlight to produce hydrogen solves the problem of intermittent and unevenly distributed sunlight by storing the solar energy in a form that can be transported to provide fuel for combustion or a future generation of fuel cell vehicles and for electricity generation at night.

The problem is that no known material can efficiently and cheaply photoelectrolyze water and be stable under illumination in an electrolyte solution for the many years necessary to justify the expensive of building a photoelectrolysis system. A number of years ago when I was thinking about this problem it became clear to me that a nanostructured oxide semiconductor had the best chance of being stable, cheap and efficient. *But which oxide?* There are about 60 metals in the periodic table and the special properties of stability, light absorption over a large part of the solar spectrum and catalytic evolution of hydrogen and oxygen would, in my view, require a complex multi-component oxide material much like the high T_c superconductors, where the record high temperature superconductors contain four or five metals. Given the large number of possible ternary or quaternary metal oxides, a combinatorial search for the holy grail of photoelectrochemistry was required.

Therefore, based, on some previous combinatorial materials techniques and some previous work where we used nitrate salts as precursors to prepare thin films of oxide superconductors, I devised a method for the fast production and screening of metal oxides for photoelectrolysis activity. The technique uses an ink jet printer to print metal oxide precursors in overlapping gradient patterns onto conductive glass substrates. Subsequent firing of the substrates at 500°C produced patterns of mixed metal oxides. The substrate with the metal oxide film is then immersed into an electrochemical cell containing an electrolyte solution. Rastering a visible light laser over the pattern, and measuring the photocurrent as a function of position, produces a false color photocurrent image of the photoelectrolysis activity in the metal oxide "library". False color representations of the photocurrent data reveal areas, associated with a particular composition, that have photoelectrolysis activity greater than Fe_2O_3 or CuO. These two elemental oxide semiconductors are printed on every substrate as internal standards since they have some activity for photoproduction of oxygen and hydrogen respectively. (see figure 1)

At this point in our research I realized that this research design is extremely simple and inexpensive and, given the large number of possible materials to be printed and screened, that there was an enormous amount of work to do. I thought getting some undergraduates involved in the project would be useful but then realized that there are potentially a large number of students who might be interested and not just at Colorado State University, my home institution at that time. After all, it is the young people who have their future prosperity at stake if energy and climate change problems are not addressed. So the idea of a "distributed research project" was born where a simple and inexpensive printing and screening kits would be developed to distribute to willing young scientists. This project is unlike other distributed research projects, such as SETI and Folding@home, since it engages the hands and minds of the participants and not just their spare computing power.

The kits needed a simple, inexpensive and flexible apparatus to facilitate the involvement of a large number of students. Since I have teenage children, I was aware of the Lego Mindstorms® sets, configurable and programmable building sets made by Lego that contain motors, gears shafts etc, and since they are a consumer item, were not nearly as expensive as scientific equipment. Many young people interested in science and engineering already have experience in robotics competitions using these kits. The photo in Figure 2 shows a laser scanner that uses an inexpensive green laser pointer and mirrors moved with Lego motors for x and y rastering of the beam over the printed and fired sample plates. The Lego laser scanner was designed and built by students working in my lab and does the same job as a system costing many thousands of dollars that we use in our research. Initial testing of our concept was done in an undergraduate research laboratory course with an enrollment of four dedicated freshman chemistry majors who were willing test subjects for this educational concept. The students learned about photoelectrochemistry, constructed their Lego apparatus and printed and screened metal oxide compositions. Several of them discovered some promising compositions and even seemed to enjoy doing it (albeit there was some self selection for motivated students given the lab was on Friday afternoon from 3-6 PM)!

After several years of attempts to get this idea externally funded, we obtained a seed grant from the Camille and Henry Dreyfus Foundation allowing us to develop our "beta" kits. In May 2008 we assembled kits containing all the necessary components for producing and screening libraries of metal oxides for water photoelectrolysis activity. (The project has been termed "The SHArK Project" for Solar Hydrogen Activity research Kit - see logo at beginning of the article). The kits contain a Lego Mindstorms® kit with a some extra Lego parts needed to construct the laser scanner, a green laser pointer, an electronics box that plugs into a USB port allowing for computer control of the electrode potential, collecting photocurrent data and for switching the laser on and off, a simple electrochemical cell constructed from plate glass, laser safety goggles, empty ink jet cartridges, software developed to control the laser scanner and assorted supplies for supporting the ink jet printer. (See Figure 2) We estimate the kits cost about $850 each (not including the ink jet printer, the computer and a laboratory furnace). We distributed 10 of these beta kits to undergraduate researchers across the country to test over the summer and fall of 2008. With the valuable experience we obtained from our summer "beta" program, we are actively working to improve the protocols and reduce the cost of the kits. We are also designing a simple furnace capable of 500°C that can be included for participants that don't have access to such a furnace. We are also expecting that the ingenuity of the enthusiastic undergraduates will produce innovative low-cost solutions for some of the remaining problems. A web site (www.thesharkproject.org) was created for the young researchers to communicate with each other and to give them access to our data base of previously tested compositions and for them to upload their own data. Recently we have been fortunate to be included in a large multi-institutional NSF-funded Center for Chemical Innovation entitled "Powering the Planet" also aimed at solar photoelectrolysis and for the next five years this center will be our instrument for further development, testing and distribution of our kits.

Realistically, discovery of a stable oxide semiconductor that can efficiently photoelectrolyze water is only the beginning of the solution to building a large-scale photoelectrolysis system that is economically viable. The students, who may be working at a small primarily undergraduate institution or even a high school, will not have access to the sophisticated analysis tools required to adequately determine the structure, electronic properties and stoichiometry of their discovery. In addition, the morphology of the oxide semiconductor in a practical device will undoubtedly involve nanostructuring to overcome the limitations of poor optical absorbance and carrier transport inherent in most oxide semiconductors, again requiring sophisticated synthesis and analysis tools. Industrial, government and academic materials research laboratories will have to be recruited to assist with the follow-up on promising materials. Indeed we found that a full year or more of graduate student time can be spent on even a cursory initial follow-up study of a new potential photoelectrolysis material. We hope to eventually be able to offer incentives to our most successful young researchers such as a summer research experience or PhD fellowships to go to a materials laboratory to follow up on their own discoveries.

We feel that the SHArK project is unique in that it engages the hands and minds of young people to learn about and participate in actual research to help solve a global scale problem that has largely been thrust upon them. In addition they will also be learning about, among other things, solid-state chemistry, semiconductor physics, solar energy conversion, electrochemistry and performing scientific research. In fact these young people will have a real opportunity to discover a material that can make a difference in the future of energy production and storage where a mix of renewable energy options will include photoelectrolysis panels that produce hydrogen from sunlight and water. Perhaps clever people can devise other distributed research programs to use budding scientific talent to attack other pressing scientific and societal problems.

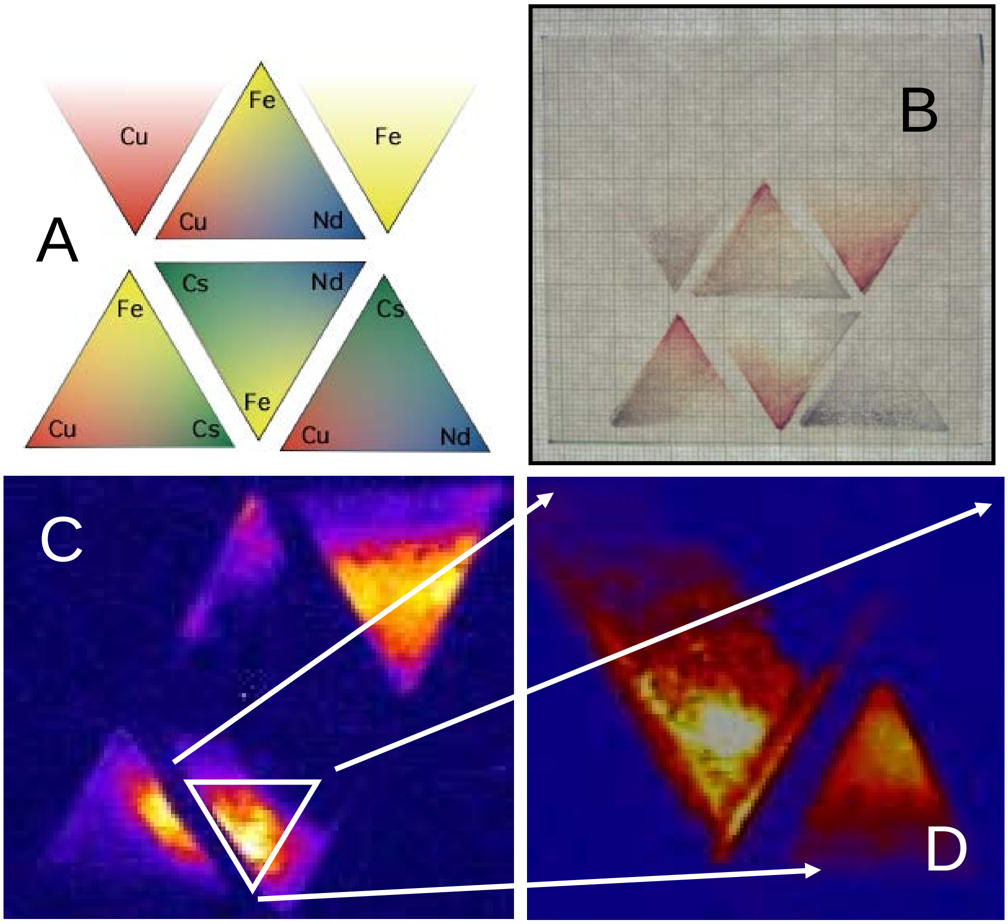

Figure 1. Printing and screening a four-metals-three-at-a-time pattern and a compositional zoom for a Fe-Cs-Nd-Cu system. A. False color template showing the positions and gradients used for printing the four metal precursor solutions. B. Photograph of the printed and fired film. Note the triangular internal standards of α-Fe_2O_3 and CuO (upper right and left, respectively) with thickness gradients (bottom to top) that are used as internal standards. C. False color photocurrent image of the film shown in B using 514.5-nm illumination under 0.5 V bias in a 0.5 M NaOH solution. The photocurrent produced at a particular "pixel", relative to the others in the two-dimensional array, is represented by its relative brightness with the most photocurrent in a particular direction (water oxidation in this case) being the brightest. D. Photocurrent scan at 514.5-nm of a triangular composition zoom in on the brightest area of the Fe-Cs-Nd triangle shown in C that has a maximum IPCE value approximately twice that of the α-Fe_2O_3 internal standard (smaller triangle to the lower right). Expanding the printing gradients within the brightest region of the n-type material created the "zoom in". Reproduced, with permission, from reference Chem. Mater. 2005, 17, 4318-4324.

Figure 2. S.H.Ar.K. Kit Items distributed to participating undergradute institutions.