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Summary: Jennifer Schmidt ’12, and Ryan Koehn ’11, conduct theoretical chemistry research as part of a solar cell research project funded by an IREE grant.

(June 18, 2010)-This summer, University of Minnesota, Morris students Jennifer Schmidt ’12, St. Cloud, and Ryan Koehn ’11, Willmar, are conducting theoretical chemistry research as part of a solar cell research project overseen by chemistry professors Joe Alia and Ted Pappenfus. Supported by an Initiative for Renewable Energy and the Environment (IREE) grant, the students are using a new computerized method to test the energy levels of polymers as phase one in the project.

What is the new method?
The solar cell research is a project focusing on creating better and more efficient renewable energy technology. Solar cells are currently comprised of silicon, which is a relatively heavy material. The Morris students are researching novel polymers that can be deposited as a film in a solar cell instead of silicon. Using polymers would be beneficial because they would be less expensive to produce and are thinner, according to the students. Schmidt and Koehn are specifically researching the distinctions in energy capturing capacities between different polymers, by using methods in theoretical chemistry, to get an idea of which polymers would be most effective for an ideal design.

Theoretical chemistry “uses principles of quantum mechanics and applies them to research questions in chemistry,” explains Schmidt. “Typically research questions being tested by theoretical chemistry are difficult to test in lab, which is why theory must be used.”

The students’ test their method by using computers to find the energy gap of the polymer. “We are calculating band gaps for conducting polymers used in solar cells,” says Koehn. The students test the differences between the energy of an electron in the polymer before and after the electron absorbs light. This is called the band gap, and each material has a different one. When the researchers find the right band gap, the solar cell will be most efficient in converting the energy of the light into electrical energy.

The second part of the students’ research is reading literature to find certain polymers’ efficiency levels. They then use a computer program, Gaussian, to run a calculation method known as Periodic Boundary Conditions (PBC). They test their method by comparing the PBC values they calculate with preexisting values in literature.

What is the goal?
If Schmidt and Koehn’s project is successful, good things could come about. Conducting this renewable energy research opens doors for future research. “In the long run, if the method we are researching is more efficient, it will decrease computational time for researchers,” Schmidt explains.

Schmidt and Koehn’s research also hopes to shed some light on the solar industry. If their research on the polymers proves their theory, it would not only be a lighter, more efficient way to capture energy, it would be a money saving
technology. Schmidt claims, “It is plausible to imagine entire roofs on top of houses covered in a thin solar cell made from polymers.”

In addition to looking for ways to change the world of renewable energy, the students also gain personal benefits from the UMM research. “I feel like the opportunities to do research here are a great stepping stone for research I’d like to do in the future at graduate school,” says Koehn.

Professor Alia sees the research opportunities as an impactful part of a UMM education. “Long term, people who are students now will be responsible for developing the technology of the future and for educating the next generation of scientists after them,” he reflects.

Phase two of the research begins the first week of July, when University of Minnesota, Morris student Mathew Lovander ’11, Willmar, conducts the synthetic, or wet, chemistry research in the lab.

Koehn calculates the energy level of a polymer.

Photo credit: Kasey Sands ’13

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