Understanding how monomer sequence affects conductance in 'molecular wires'

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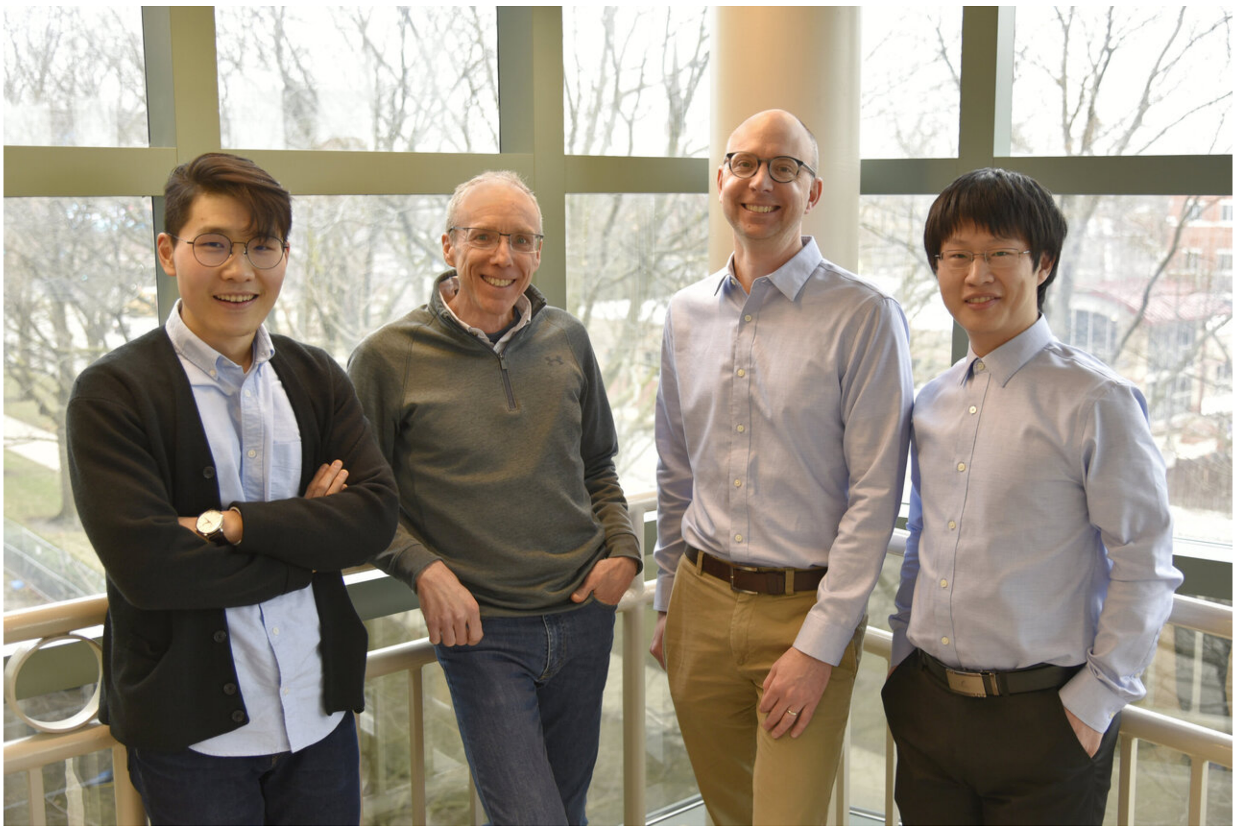

Researchers in the Schroeder and Moore groups at the University of Illinois are interested in building and studying chain molecules with high levels of precision. Pictured from left, Hao Yu, graduate student in chemical and biomolecular engineering; Jeff Moore, professor of chemistry; Charles Schroeder, professor of chemical and biomolecular engineering; and Songsong Li, graduate student in materials science and engineering. Credit: Doris Dahl, Beckman Institute, University of Illinois at Urbana-Champaign

Researchers in the Schroeder and Moore groups at the University of Illinois at Urbana-Champaign have published a new study that illustrates how changes in the polymer sequence affect charge transport properties. This work required the ability to build and study chain molecules with high levels of precision.

The paper, "Charge Transport in Sequence-Defined Conjugated Oligomers," was published in the *Journal of the American Chemical Society*.

Chain molecules or polymers are ubiquitous in modern society, with organic electronic materials increasingly used in solar cells, flat panel displays, and sensors. However, conventional materials are generally made by statistical polymerization, where the order of the subunits or monomers—the monomer sequence—is random.

"Traditional polymerization methods do not give us a perfect level of control of sequence," said Charles Schroeder, the associate head and Ray and Beverly Mentzer Professor in Chemical and Biomolecular Engineering and a full-time faculty member at the Beckman Institute for Advanced Science and Technology. "As a result, it has been challenging to ask how the monomer sequence affects its properties."

The researchers developed a method called iterative synthesis to deal with the problem. "Protein synthesis in our cells occurs by adding the amino acids one by one. We use the same method for making synthetic polymers where we add distinct monomers in a one-by-one fashion. This allows us to precisely control the sequence in a linear arrangement," said Hao Yu, a graduate student in the Schroeder Group, and the Moore Group led by Jeff Moore, the Stanley O. Ikenberry Endowed Chair and professor of chemistry.

After making the materials, the researchers studied their charge transport properties using single molecule techniques. In this way, they were able to measure the conductance through single chains, much like a 'molecular wire.'

"Molecular wires are generally good at transporting charge," Schroeder said. "We wanted to know how the charge transport properties change if the overall sequence changes."

Yu added molecular anchors at both ends of the chain molecule to enable the characterization. "We used a technique called the scanning tunneling microscope-break junction method, where the anchors link to two gold electrodes and form a molecular junction," said Songsong Li, a graduate student in the Schroeder Group. "Then we impose an applied bias or voltage across the molecule, and this allows us to measure the charge transport properties of these polymers."

"Currently the synthesis method is labor intensive," Schroeder said. "Moving forward, we are developing automated synthesis methods in the Beckman Institute to generate large libraries of sequence-defined molecules."

"The implications of this work are significant," said Dawanne Poree, program manager at the Army Research Office that supports the work. "It's often been wondered if the sequence-dependent properties observed in biological polymers could translate to synthetic polymeric materials. This work represents a step toward answering this question. Additionally, this work provides key insights into how molecular structure can be rationally designed and manipulated to render materials with designer properties of interest to the Army such as nanoelectronics, energy transport, molecular encoding, and data storage, self-healing, and more."

More information: Hao Yu et al, Charge Transport in Sequence-

Defined Conjugated Oligomers, *Journal of the American Chemical Society* (2020). DOI: 10.1021/jacs.0c00043

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