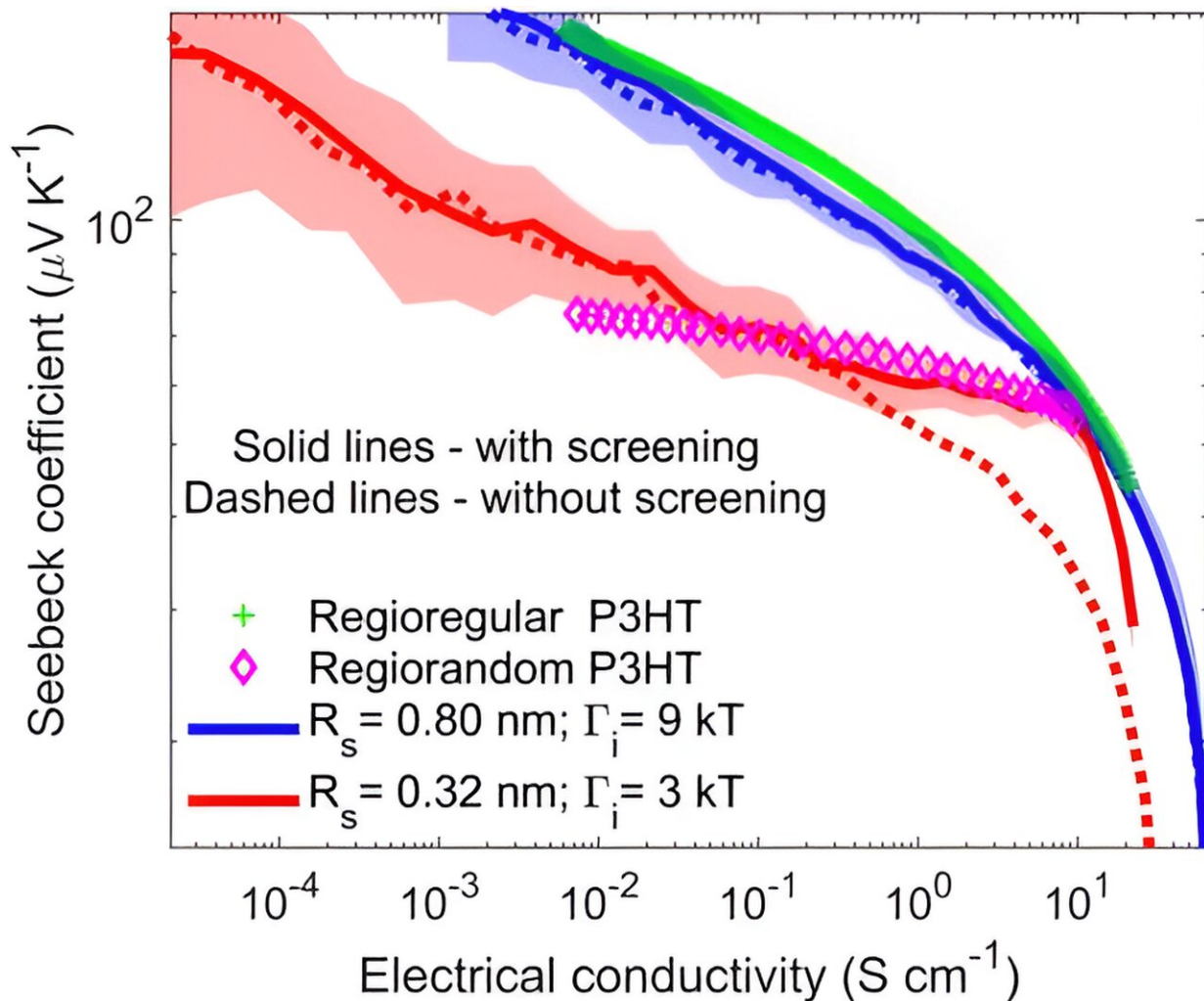


Uncovering the physics of how electrons screen against conductivity-killer in organic semiconductors

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Seebeck coefficient against electric conductivity measurements of RR and RRA-P3HT doped with iodine and measured while dedoping. We took $R_d = 0.21 \text{ nm}$

to match the radius of iodide anion ($R_I = 0.206 \text{ nm}$). Dashed lines correspond to the case without screening, while bands around simulation results represent variance from randomly sampling the energy sites. The attempt-to-hop frequency is 34 for RR and 10 THz for RRa P3HT.

California's Silicon Valley and Utah's Silicon Slopes are named for the element most associated with semiconductors, the backbone of the computer revolution. Anything computerized or electronic depends on semiconductors, a substance with properties that conduct electrical current under certain conditions. Traditional semiconductors are made from inorganic materials—like silicon—that require vast amounts of water and energy to produce.

For years, scientists have tried to make environmentally friendly alternatives using organic materials, such as polymers. Polymers are formed by linking [small molecules](#) together to make long chains. The polymerization process avoids many of the energy-intensive steps required in traditional semiconductor manufacturing and uses far less water and fewer gases and chemicals.

They're also cheap to make and would enable flexible electronics, wearable sensors, and biocompatible devices that could be introduced inside the body. The problem is that their conductivity, while good, is not as high as their inorganic counterparts.

All electronic materials require doping, a method of infusing molecules into semiconductors to boost conductivity. Scientists use molecules called dopants to define the conductive parts of electrical circuits. Doping in organic materials has vexed scientists because of a lack of consistency—sometimes dopants improve conductivity while other times they make it worse.

In a new study, researchers from the University of Utah and the University of Massachusetts Amherst have uncovered the physics that drive [dopant](#) and polymer interactions that explain the inconsistent conductivity issue.

The team discovered that positively charged carriers pull negatively charged dopants from the [polymer chains](#), preventing the flow of electrical current and tanking the material's conductivity. However, their experiments revealed that when enough dopants were injected into the system, the electrons' behavior changed to act as a collective screen against the attractive forces, allowing the rest of the electrons to flow unimpeded.

"The ideal case would be to dump a bunch of [free electrons](#) into the material to do the work of conducting. Of course, we can't—we have to use molecules to supply the electrons," said Zlatan Akšamija, associate professor of materials science and engineering at the U and lead author of the study. "Our next step is to find the dopant/organic material combinations that can weaken that interaction and make the conductivity even higher. But we didn't understand that interaction well enough to be able to tackle it until now."

The [study](#) is published in the journal *Physical Review Letters*.

Doping juices conductivity

Electricity is a flow of electrons. Silicon on its own is a bad conductor—four electrons in the outer orbital form perfect covalent bonds with nearby silicon atoms, leaving no free electrons. Here's where doping comes in. Adding an impurity to the silicon can do two things: Contribute extra electrons into the system or reduce electrons in the system, creating positively charged carriers called holes.

For example, arsenic is a common dopant because it has five electrons in its outer orbital—four will bond to the silicon and the fifth will remain free. Eventually, the dopants will contribute enough free electrons to allow an electrical current to flow through the silicon.

Unlike silicon, organic materials have a disordered structure in their polymer chains, resulting in complicated interactions between the dopant's extra electrons and the polymerized material, Akšamija explained.

"Imagine polymers are a bowl of spaghetti. They don't really stack perfectly. Because of that, the electrons are forced to hop from one part of the polymer to another and onto the next chain, pushed along by voltage," he said.

Each dopant contributes one electron into the system at a time, which means that, at first, the electrons that hop through the polymer are diluted. If an electron is hopping along the chain and passes near a dopant, the opposite charges will attract each other and cause the electron to veer off course and disrupt the electrical current.

The revelation of this study was finding that this behavior changed with a critical mass of electrons in the system—when a threshold is passed, the mob of electrons collectively respond. When a group of electrons pass a dopant, some are pulled towards the charge and create a screen that blocks the rest of the electrons from feeling the interaction.

"And that's where the screening is really doing the work of blocking the dopants. The carriers are screening the dopants away, which makes it easier for other carriers to hop around more efficiently. This paper describes the physical mechanism by which this happens," said Akšamija.

Experimentation and theory

The UMass Amherst chemists ran the physical experiments. They used two types of polymers that had structures that were more and less disordered. They then used a solvent and coated it onto a thin layer of glass. They then doped the polymer with iodine vapors. One benefit of iodine is that it's unstable—over time, the polymer gradually loses dopant molecules to evaporation.

"This was useful for experiments because we can keep measuring the conductivity of the polymer over the period of 24 or 48 hours. This protocol gives us a curve of conductivity as a function of how many dopants are left in the material," said Dhandapani Venkataraman, professor of chemistry at UMASS Amherst and co-author of the study.

"It's a neat trick to get access to almost four orders of magnitude of change in conductivity from low, medium versus high concentrations of dopants ... all the way down to being essentially back to its original pristine insulating state."

The chemists ran experiments on two different versions of the same polymer—one that was more regular and the one that was more disordered. They could then compare the conductivity in the two polymers as the dopant concentration changed.

"At first, we were puzzled by some of the experimental results, especially when we had a large number of dopants. We expected that the disordered polymer would be very inferior to the ordered polymer at all concentrations of the dopants. But that was not the case," said Venkataraman.

Akšamija's research group focused on the interactions of the materials. They were able to contrast the different instances of the same polymer

with larger or smaller amounts of disorder to discern where screening was happening.

This screening behavior had never been considered as a part of organic semiconductor systems, so they dug out paper and pencils to understand how molecules and charges interact using the first physics principles: What is the underlying equation that governs the interaction of charges? Akšamija's lab started there and built it back up. They then translated the formulas into code that simulated the hopping of electrons in the presence of dopants while including the screening behavior.

"We had finally converged to the point where the [computer simulations](#) can really capture the experiments, not just qualitatively, but really quantitatively. The only way to get the simulation and the experiments to line up was when we included this effect of screening," said Akšamija.

Currently, the authors are employing [artificial intelligence](#) to help discover new combinations of polymers and dopants that could yield the highest [conductivity](#).

More information: Muhamed Duhandžić et al, Carrier Screening Controls Transport in Conjugated Polymers at High Doping Concentrations, *Physical Review Letters* (2023). [DOI: 10.1103/PhysRevLett.131.248101](#). *OnarXiv* : [DOI: 10.48550/arxiv.2311.03726](#)

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