# Solitonics in molecular wires could benefit electronics

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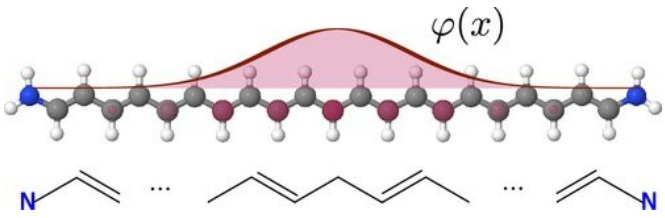


Chemical structure of polymethine – the polyacetylene molecules considered in this work. Corresponding Kohn?Sham orbital that forms the topologically protected domain-wall state in a wire (top) and the resonant configuration for an uncharged neutral molecule (bottom). Credit: *Nano Letters*

Soliton descriptions for the conducting polymers polyacetylene—descriptions based around a type of solitary wave—caused great excitement when they first broke in the seminal reports by Su, Schrieffer, Heeger (SSH) and Kivelson over 30 years ago. As some of the simplest topological insulators, these molecules are now attracting revived interest. However, problems synthesizing single polyacetylene molecules had limited these soliton studies to extrapolations of soliton characteristics from averages over large numbers of soliton-bearing molecules, which is quite indirect. Reports of synthesis and characterization of single polyacetylene molecular wires in 2019 changed this. Now, calculations by researchers in Germany and the U.S. have identified how the solitons in these single molecular strands behave, pointing to a level of soliton control—"solitonics"—that could be useful to electronic devices and sensors.

Solitons occur where nonlinear and dispersive effects cancel so that a solitary wave packet becomes self-reinforcing. They have a number of particle characteristics in the way they maintain a constant shape and emerge from collisions unchanged. In optical wave guides, the nonlinear contribution is proportional to intensity, producing wave self-focusing so that the wave passes through space and time unchanged. However, the self-preserving soliton feature can also be associated with a change in bond order such as a kink or domain wall. Solitons emerge in descriptions of polyacetylene molecular wires on account of the different domains these wires can have.

Polyacetylene molecules alternate between single and double bonds along the chain, and the order of these bond types defines different domains. The soliton is a way of describing the domain wall between sections of the chain that have different ordering. The domain wall can move but its shape remains the same. It is also very light—around six times an electron mass—yet it may distort the lattice and move heavier nuclei as it ripples through.

The researchers led by Daniel Hernangómez-Pérez and Ferdinand Evers at the University of Regensburg in Germany, in collaboration with researchers at Columbia University in the U.S., applied density functional theory calculations to polyacetylene to see how these solitons behave in single wires. "One of our primary motivations is understanding what type of topological properties can be observed at the single-molecule level in realistic scenarios," explains Hernangómez-Pérez.

**Electronics meets solitonics**

They found that it was possible to control the position of the soliton through the chemical entities at either end of the molecular chain. The soliton can be charged with no spin or charge free but with a spin of one-half. For charged solitons, the researchers show that applying an electric field can further manipulate the position of the soliton on the molecular chain, which can be observed through polarization measurements or changes in conductance. The conductance changes exponentially when the soliton moves towards the edge, which as Hernangómez-Pérez suggests provides a sensitivity that could be useful for

detecting electrical fields.

A perhaps unexpected result occurs when the soliton has reached one end of the chain and the field is ramped up further. Instead of some sort of dielectric breakdown, an additional soliton-antisoliton pair forms, releasing electrostatic energy.

**Further solitonic potential**

Although researchers have already shown that it is possible to synthesize single polyacetylene molecular wires long enough to harbor solitons, other challenges remain. They will need to establish a way of ensuring the wire retains the excess charge for a charged soliton, as well as how to chemically attach the right chemical end groups and subject the soliton to in-plane electric fields. However, Hernangómez-Pérez does not see any of these issues as insurmountable. For instance, the in-plane field could be provided by metallic adatoms deposited with a scanning near-field microscope.

As for his own line of future research, Hernangómez-Pérez lists a number of outstanding theoretical issues to tackle: "There are several possibilities: (i) understanding the role of the substrate and possible lattice mismatch between the substrate and polyacetylene chain; (ii) investigate using theoretical tools such as density-functional theory inter-chain coupling or how creation of solitons on one chain might affect neighboring chains; (iii) investigate theoretically domain-wall formation in similar carbon-based molecules."

So far, the researchers' calculations do not extend to the behavior of a zero-charge polyacetylene soliton that carries spin, but they expect that it should be possible to manipulate this with a magnetic field gradient. "In principle, one could think of spin currents along the wire in the same way as electrical currents," suggests Hernangómez-Pérez. "But it is very premature to talk about any impact of this for spintronics."

**More information:** Daniel Hernangómez-Pérez et al. Solitonics with Polyacetylenes, *Nano Letters* (2020). DOI: 10.1021/acs.nanolett.0c00136