

Research Highlights

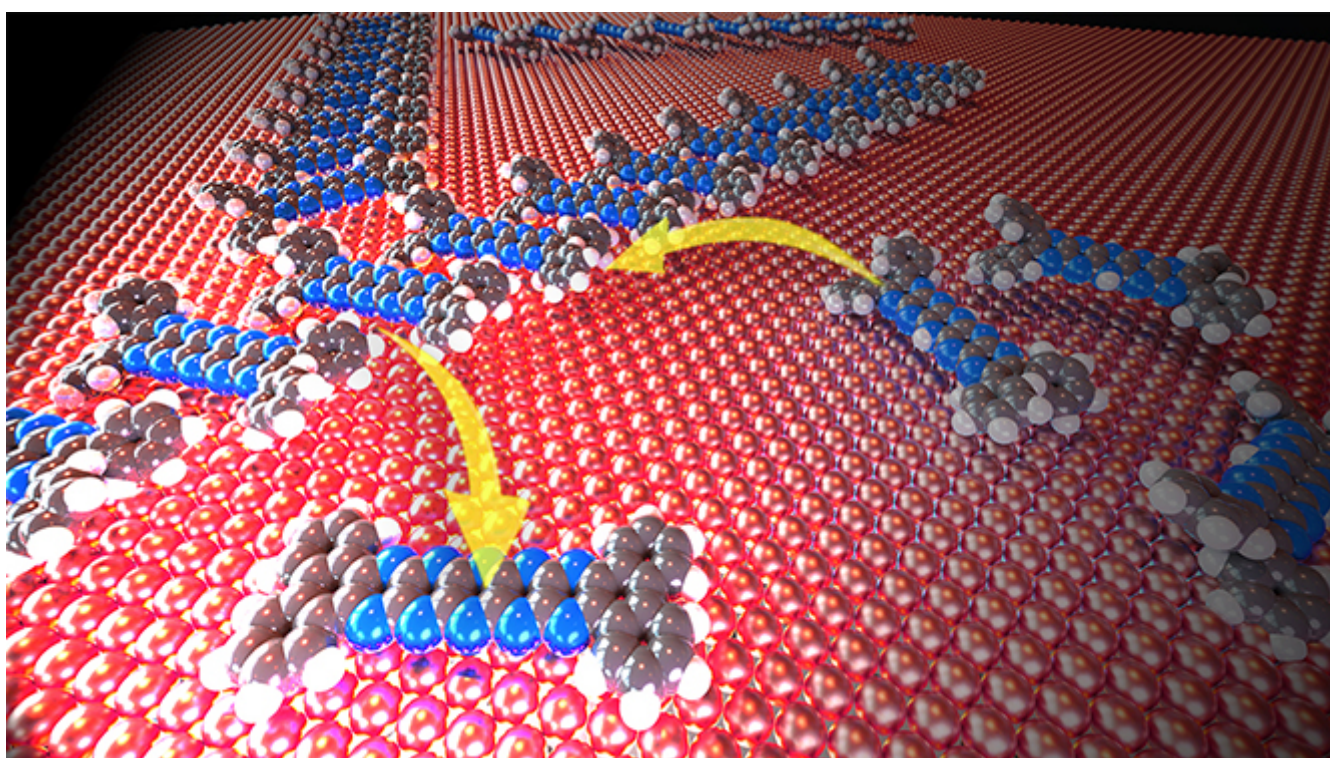
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“On-Surface Shapeshifters” Exhibit Oxidation-State-Dependent Conformational and Self-assembly Behaviors

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A team at MANA has found that substances known as pyrazinacenes exhibit on-surface oxidation-state-dependent conformational and self-assembly behaviors. This “shape-shifting” could result in a variety of applications.



The team’s broad experimental and theoretical study revealed that pyrazinacenes containing decaazapentacene are stable against oxidation but unstable against reduction.

Pyrazinacenes represent an unusual class of redox-active chromophores, and represent an emerging class of highly nitrogenous heteroacenes with unique properties. They have excellent potential for use based on their special supramolecular properties, including interactions in biological systems. They lie at the core of molecular materials’ applications because of their important optical and electronic features.

The team determined that the already established structure-function relationships of molecular materials known from solution now need to be re-evaluated to predict and understand the interface-specific chemical, electronic, optical and mechanical properties of any newly synthesized molecules.

The research was completed by David Miklík (WPI-MANA) and S. Fatemeh Mousavi (Department of Physics, University of Basel, Switzerland) under the leadership of Thomas Jung (Laboratory of Micro- and Nanotechnology, Paul Scherrer Institute, Switzerland) and [Jonathan P. Hill](#) (WPI-MANA).

"We suggest the term 'on-surface shapeshifter' to describe these compounds, based on their oxidation-state-coupled on-surface molecular morphology variations," the scientists said in their paper.

The substances' chemical complexity, they said, motivates further investigations comparing in-solution and interfacial reactivity, in particular toward tunable photo-redox compounds or the generation of synthetically inaccessible molecules.

This research was carried out by David Miklík of the Functional Chromophores Group of WPI-MANA and S. Fatemeh Mousavi of the University of Basel, Switzerland, and their collaborators.

Reference

"Pyrazinacenes Exhibit On-Surface Oxidation-State-Dependent Conformational and Self-Assembly Behaviours"

David Miklík, S. Fatemeh Mousavi, Zuzana Burešová, Anna Middleton, Yoshitaka Matsushita, Jan Labuta, Aisha Ahsan, Luiza Buimaga-Iarinca, Paul A. Karr, Filip Bureš, Gary J. Richards, Pavel Švec, Toshiyuki Mori, Katsuhiko Ariga, Yutaka Wakayama, Cristian Morari, Francis D'Souza, Thomas A. Jung and [Jonathan P. Hill](#)

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