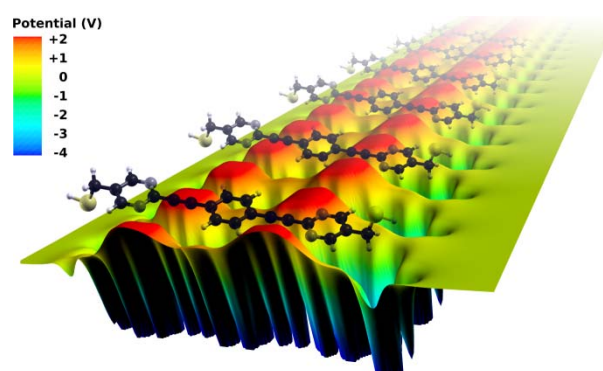


Molecules working together in new ways: Cooperative electrostatic effects can dominate charge-transport phenomena in self-assembled monolayers

The ultimate miniaturization of (opto-)electronics lies in individual molecules performing the functions usually attributed to silicon-based devices, such as switching electrical current. As reliably “wiring up” individual molecules has proven difficult, using monomolecular layers instead is technologically more promising. Usually, however, the chemical design of the constituting molecules still proceeds with the properties of a single one in mind, because most direct intermolecular interactions are weak. During his research stay at the Humboldt-Universität, IRIS Adlershof - sponsored visiting scientist David Egger showed that this approach can lead to surprises. He demonstrated that even the most basic property of any electronic device, the current passing through at a given voltage, can differ drastically between monolayer devices made from almost identical molecules that exhibit virtually the same electronic properties when considered individually. The key lies in how exactly charge is distributed among the atoms within the molecules. The resulting electrostatic fields, while negligible for a single molecule, can add up in tightly packed layers, thus indirectly affecting their charge-transport properties.

Considering these cooperative electrostatic effects in molecular design for future monolayer devices will enable

better control over their functionality and performance.



The collective electrostatic action of dipolar bonds at both ends of the molecules raises the electrostatic potential in the center of the monolayer (red region). Thereby, the quantum-mechanical states through which current can flow are lifted up in energy to more favorably align with those of external metal electrodes.

Polarity Switching of Charge Transport and Thermoelectricity in Self-Assembled Monolayer Devices

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