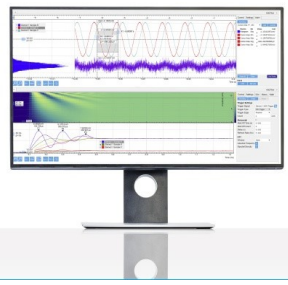
The Journal of Chemical Physics

Preface: Special Topic on Frontiers in Molecular Scale Electronics

Cite as: J. Chem. Phys. **146**, 092101 (2017); https://doi.org/10.1063/1.4977469
Submitted: 13 February 2017 . Accepted: 13 February 2017 . Published Online: 02 March 2017

Ferdinand Evers, and Latha Venkataraman



Preface: Special Topic on Frontiers in Molecular Scale Electronics

Ferdinand Evers[1,a)] and Latha Venkataraman[2,a)]
[1]*Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany*
[2]*Department of Applied Physics and Department of Chemistry, Columbia University, New York, New York 10027, USA*

(Received 13 February 2017; accepted 13 February 2017; published online 2 March 2017)

The electronic, mechanical, and thermoelectric properties of molecular scale devices have fascinated scientists across several disciplines in natural sciences and engineering. The interest is partially technological, driven by the fast miniaturization of integrated circuits that now have reached characteristic features at the nanometer scale. Equally important, a very strong incentive also exists to elucidate the fundamental aspects of structure-function relations for nanoscale devices, which utilize molecular building blocks as functional units. Thus motivated, a rich research field has established itself, broadly termed "Molecular Electronics," that hosts a plethora of activities devoted to this goal in chemistry, physics, and electrical engineering. This Special Topic on Frontiers of Molecular Scale Electronics captures recent theoretical and experimental advances in the field. *Published by AIP Publishing.* [http://dx.doi.org/10.1063/1.4977469]

Over the past decade, *molecular electronics* has witnessed tremendous experimental and theoretical advances, brought about primarily by the collective effort of leading scientists. The collection of articles presented in this special topic issue indicates the state of this field. It demonstrates the breadth of topics being investigated and offers a survey that highlights some of the latest developments and the related prospects. We hope that it can serve as an introduction into a field that is as complex and diverse as it is exciting for the young.

The focus of *molecular electronics* has been to understand and manipulate currents of charge, spin, and heat across devices that consist of a molecular wire or a chain of metal atoms connected between two electrodes. An experimental challenge lies in our ability to create such devices with atomic precision and measure their properties; given the nanometer or sub-nanometer length scales involved, this often relies on a bottom-up approach that requires repeated measurements to ensure reproducibility. The experimental works published in this special edition represent the most significant measurement techniques; they also discuss important aspects of data analysis critical to drawing conclusions about the structure and electronics of single-molecule devices.[1–5] Furthermore, a variety of physical phenomena are encountered when a current flows through a molecule that leave a trace, e.g., in the current-voltage characteristics. These include aspects of electronic correlations,[6] magnetism, and spin-related effects.[7–9] Molecular vibrations, junction mechanics, and associated thermal effects have been analyzed experimentally and theoretically[10–14] and time resolved studies are also under way.[15–17]

With such a wealth of phenomena, many of which are very specific to molecular junctions, it is not surprising that the field has motivated a significant amount of theoretical work. Electronic structure effects are being investigated that might enable molecule-specific functionalities.[18–22] The Kondo-effect can become under-screened by design in atomic wires;[23] more generally speaking, on the atomic scale, quantum fluctuations are enhanced giving rise to unexpected magnetic behavior.[24] The interaction between electrons and nuclei tends to be strong in molecular matter and its consequences have been investigated intensively.[25–27] The theoretical challenge is to describe transport processes in a molecule, i.e., a genuine many-body system, that is coupled to two reservoirs. It necessitates developing new tools[28–30] and extending familiar concepts[31,32] to explore non-equilibrium phenomena inherently present when currents flow across the devices in response to an applied voltage.

After glancing through this issue, a newcomer to the field will get a first impression of *molecular electronics*, while an expert can be informed about the status of a variety of subfields. This Special Topic on Frontiers in Molecular Scale Electronics provides a significant sampling of recent work in this broad field.

[a)]Electronic addresses: ferdinand.evers@physik.uni-regensburg.de and lv2117@columbia.edu

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