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Themed collection on molecular scale electronics

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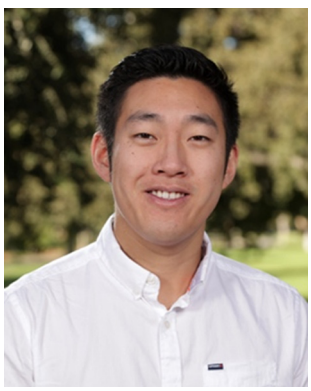
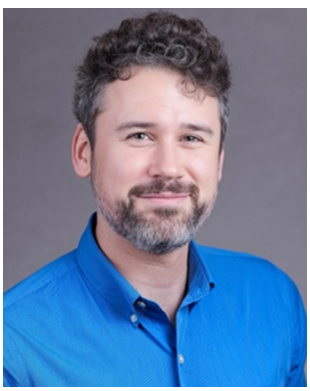
This themed collection in the *Journal of Materials Chemistry C* provides a window into the most exciting trends and questions that currently grip the field of molecular scale electronics. Interest in molecular electronics—to use individual molecules as the active elements in electronic circuitry—dates back to the 1950s, where Air Force and corporate interests aligned in a vision to make miniaturized electronics through bottom-up rather than top-down approaches, as the molecular scale represents the ultimate limit of device miniaturization.[1] In 1974, Aviram and Ratner provided the first vision for what such a functional molecular electronic component might look like in a molecular rectifier.[2] Scanning tunneling microscopy-based techniques and related approaches ultimately provided the means to rapidly characterize the electronic properties of an extensive range of molecular junctions.[3–9]

While it is still a central aspiration to make practical electronics from molecules, this is no longer the singular driving motivation for the field. New research directions have branched off from this initial goal, leading to perhaps the most interesting lines of inquiry. We can use the tools developed to probe molecular junctions for discovering novel quantum transport phenomena that emerge only at the molecular scale, achieve molecular level insight into the properties of bulk materials, and explore how concepts from physical organic chemistry or interfacial chemical reactions can be used to control quantum



Timothy A. Su

Tim Su is an Assistant Professor in the Department of Chemistry and the Materials Science and Engineering Program at the University of California, Riverside. He received his BS in Chemistry from the University of California, Berkeley in 2011 with Prof. Jean Fréchet. Tim obtained his PhD in Chemistry from Columbia University in 2016 as an NSF Graduate Fellow with Prof. Colin Nuckolls. Tim returned to UC Berkeley as an NIH Postdoctoral Fellow with Prof. Chris Chang before starting his independent career in 2019. Research in the Su lab focuses on silicon molecular materials and main group molecular electronics. His group's work has been supported by Hellman Foundation, ACS PRF, AFOSR, NSF CAREER, and Cottrell Scholar awards.



Michael S. Inkpen

Mike Inkpen is an Assistant Professor of Chemistry in the Department of Chemistry at the University of Southern California, where he started his independent career in 2019. He obtained his MChem from Durham University in 2008, and his PhD in 2013 from Imperial College London with Prof. Nicholas J. Long and Prof. Tim Albrecht. In 2015 he joined the group of Prof. Latha Venkataraman at Columbia University as a Marie Skłodowska-Curie Fellow. He returned to Europe in 2017 for the final year of his fellowship, working with Prof. Philippe Hapiot at the University of Rennes 1. Research in the Inkpen lab focuses on molecular nanoscience, studying charge transport processes and reactivity in single-molecule junctions and self-assembled surface-bound monolayers. His group's work has been supported by funding from the ACS PRF and the NSF CAREER Awards.

transport through molecules. Molecular electronics is now about so much more than whether we can make a practical molecular electronic—it has become a platform for discovering new fundamental science through the unique lens of tunneling transport.

Over the last three decades, measurement and modeling approaches have grown in both sophistication and accessibility, attracting a growing base of scientists working together across synthesis, theory, measurement, and device engineering to explore these fundamental questions, with some collaborations happening across the globe. Indeed, a diverse cohort of international researchers are featured in this themed collection.

One flavor of molecular electronics seeks to interrogate molecules forming dense self-assembled monolayers that are probed in large-area junctions. In this themed collection, Cea, Martin, and coworkers are exploring the use of transparent and flexible electrodes (**https://doi.org/10.1039/D3TC02237D**) within this context toward wearable molecular electronic devices. Meanwhile, Li and coworkers take a different approach and consider using conductive ionogels to replace conventional electrodes in large-area junctions that operate under aqueous environments necessary for bioelectronic applications (**https://doi.org/10.1039/D3TC03733A**). Finally, Lambert, J. Wang, X. Wang, Ismael, and coworkers apply stepwise assembly approaches to develop molecular arrays on graphene electrodes for thermoelectric applications (**https://doi.org/10.1039/D3TC02842A**).

It has also been appreciated how the nature of the electrode–molecule contact influences molecular conductance and mechanical stability properties. We have only explored a limited chemical space when it comes to linker group design. In this collection, Zhou, Wang, Chen, and coworkers explore how the coordination modes and denticity of triazole contact groups on gold electrodes influence single-molecule junction conductance (**https://doi.org/10.1039/D3TC03618A**). Lacroix, Sun, and coworkers investigate linker engineering through a mixed diazonium–amino linker system to create highly robust porphyrin-based single-molecule junctions, with junction lifetimes up to 70 seconds (**https://doi.org/10.1039/D3TC04142E**). Hou and coworkers apply theories to study the use of oxazine-based linkers that may serve as covalent anchors for carbon nanoelectrodes (**https://doi.org/10.1039/D3TC03720G**).

The nature of the electrode–linker contact is complex, as there are multiple ways a linker can interact with electrodes, with each leading to its own conductance signature. However, it is difficult to tease these out from a single histogram that compiles all measurement traces. Van Veen, Ornago, van der Zant, and El Abbassi describe a generalized neural network approach to separate traces that contain molecular plateaus from traces where no molecule connects in the junction to facilitate interpretation of molecular conductance measurements where the junction formation probability is low (**https://doi.org/10.1039/D3TC02346J**).

There has been mounting interest in exploring new concepts for how molecular connectivity in the molecular backbone can be used to control quantum transport. Moth-Poulsen and coworkers explore a bond connectivity switch in the norbornadiene/quadricyclane scaffold showing that thioacetate- and *tert*-butyl-terminated molecules outperform the methyl thioether-terminated ones (**https://doi.org/10.1039/D3TC02652C**). Venkatramani and coworkers computationally explore the impact of pyridyl nitrogen's *ortho*-, *meta*-, and *para*-connectivity on electronic transmission in polypyridyl molecular wires (**https://doi.org/10.1039/D3TC02651E**). Mota and coworkers computationally study how ring size and connectivity in graphene nanoribbons impact transport properties in nanodevices (**https://doi.org/10.1039/D3TC03701K**). Guo, Jia, Li, and coworkers summarize related concepts in designing non-volatile memories in single molecule devices in their review article (**https://doi.org/10.1039/D3TC03724J**).

Another emerging area is to explore how anti-aromatic backbones impact molecular junction properties, as these are expected to demonstrate heightened molecular conductance.[10,11] Here, Zotti, Leary, and coworkers computationally investigate charge transport in non-alternant antiaromatic dithienopentalenes (**https://doi.org/10.1039/D3TC04266A**). Nishino and coworkers provide new insight into the nature of π-stacking van der Waals interactions in antiaromatic molecules *via* atomic force spectroscopy in large-area junctions (**https://doi.org/10.1039/D3TC04166B**). Another area of emerging interest lies in understanding the impact of spin on molecular electronics and spintronics, particularly in organometallic complexes. Hou and coworkers model spin-polarized currents in square-planar iron complexes (**https://doi.org/10.1039/D3TC03719C**). Meanwhile,

Haixing Li

Haixing Li is an Assistant Professor in the Department of Physics at the City University of Hong Kong. She obtained her BS in Physics from the University of Science and Technology of China in 2012 where she did her undergraduate thesis with Prof. Xianhui Chen. She then moved to Columbia University and earned her PhD in Applied Physics in 2017 under the guidance of Prof. Latha Venkataraman. She worked as a postdoctoral fellow and later a Charles H. Revson Senior Fellow in the laboratory of Prof. Ruben Gonzalez at Columbia University from 2017 to 2021. Her research group examine molecules and develop measurement tools at the single molecule level to spark advances in electronics and sustainability. Her group's work is supported by an Early Career Scheme and a General Research Fund from Research Grants Council of Hong Kong.

Schneider, Feyer, Cojocariu, Carlotto, and coworkers explore the impact of π-conjugation on magnetic anisotropy in nickel tetraphenylporphyrin complexes for spintronic applications (**https://doi.org/10.1039/D3TC02726K**).

In concert, these articles highlight the diversity of research questions and approaches at the forefront of molecular scale electronics.

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