DMR-2046483

CAREER: Mitigating Detrimental Vibrational Effects in Organic Semiconductors

Michael T. Ruggiero, University of Vermont & State Agricultural College

Organic semiconductors hold immense potential for revolutionizing electronic devices, offering applications from flexible electronics to translucent solar cells. To facilitate this technological advancement, it is imperative to understand the fundamental factors influencing both favorable, and unfavorable, performance – at the atomic/quantum level. In our 2023 research supported by DMR funding, we made important progress towards these goals:

1. **Identifying an Unsuitable Class of Molecules:**
    1. A comprehensive investigation revealed that a class of molecules, extensively studied by the community, proved unsuitable for advanced electronics due to fundamental reasons. This critical insight redirected focus towards more promising materials.
    2. This work was featured on the front cover of the prestigious peer-reviewed journal, *ChemComm* (Fig 1a), where it was highlighted for prompting a shift in research efforts.

2. **Quantum-Mechanical Analysis of Atomic Influence on Semiconducting ability:**
    1. Employing careful quantum-mechanical analysis, we delved into the influence of individual atoms in organic electronics (Fig 1b).
    2. This analysis uncovered unprecedented insights into the design of new materials for advanced electronic applications, considering atomic motions (Fig 1c).
    3. Our groundbreaking work, published in the leading journal *Advanced Functional Materials*, provides a roadmap for designing superior organic semiconductors.

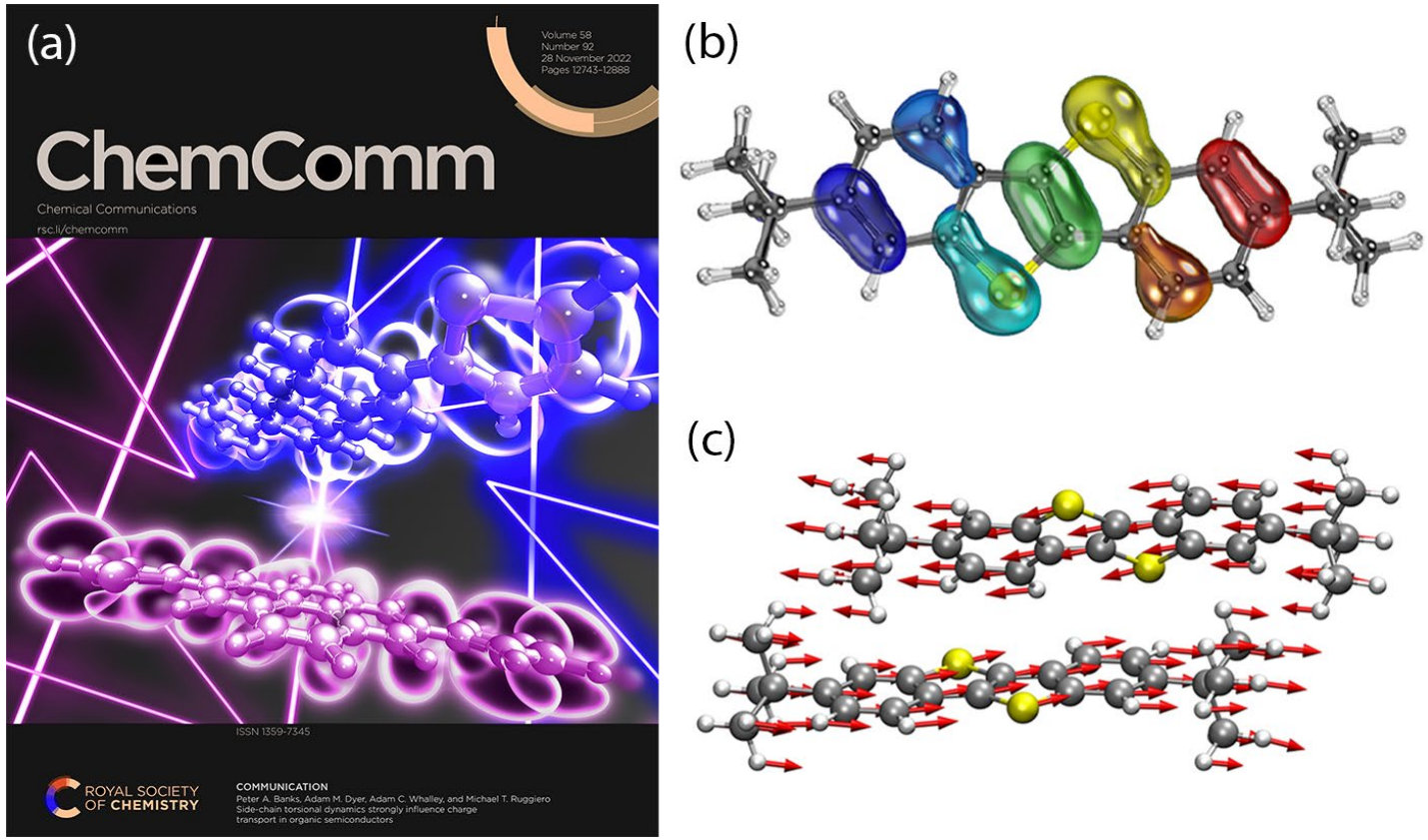

Figure 1. (a) Front cover of *ChemComm* highlighting the PI's work understanding vibrational effects in organic electronics. (b) lobes of electron density in an organic semiconducting molecule relevant to charge transport. (c) Detrimental vibrational motions, with the molecular motion indicated by red arrows.

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As part of this DMR-funded project, the principal investigator is working with underrepresented students in inner-city schools to highlight chemistry and optics concepts to K-12 students.

In 2023, the PI and his team volunteered at an inner-city school in Rochester, NY (Pinnacle School, School #35). This year, they worked with a first-grade classroom (6-7 year olds) to highlight the 'magic of chemistry'. The DMR-funded team supervised two hands-on experiments with students, where the students were free to explore on their own in a guided fashion. Students were taught to ***think*** about their observations, and to ***ask questions*** about what they were observing, in order to teach students analytical skills and to get them excited about STEM projects.

The day was a great success, and more events are planned at more schools with additional age groups in calendar year 2024.