Portland State
Chemistry

College of Liberal Arts and Sciences
Spring 2021 Chemistry Seminar Series
Friday, April 2nd

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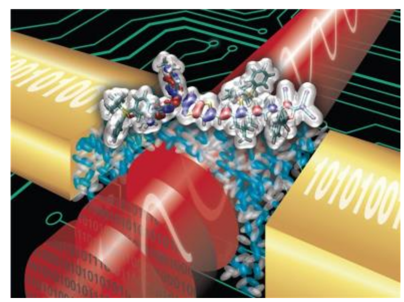
Hybrid Organic Electro-optics: Computational Chemistry to Commercialization

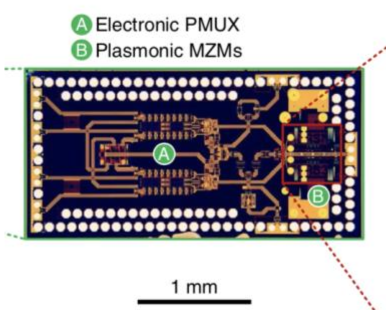
Computing and telecommunications are presently undergoing a massive transformation. Performance growth from specialization and connectivity has replaced the general-purpose growth of the last few decades, with particular emphases on sensing, ML/AI, and the Internet of Things/Edge computing. These trends require rapid signal processing and large interconnect bandwidths at distances ranging from long-distance networks to between modules within individual chips. Optical (photonic) computing technologies can deliver exceptional performance for these applications, shrinking technology used for fiber optics down to the chip scale, but cost-and power-efficient implementation requires compatibility in size, voltage, and processing techniques with CMOS electronics.



Schematic of light and OEO material interacting in a plasmonic waveguide (Xu et al. 2021)

Organic electro-optic (OEO) materials integrated in hybrid device architectures, such as plasmonic-organic hybrid (POH) and silicon-organic hybrid (SOH) photonics systems present a promising approach that leverages the exceptional performance of organic chromophores in controlling the propagation of light via rapid changes in their refractive index.

We have developed and applied computational tools for designing future generations of electro optic materials with unprecedented performance and applied these tools towards development of multiple families of novel OEO materials. Understanding these materials and designing for high performance requires multi-scale modeling techniques, ranging from electronic structure calculations and quantitative structure-property relationships during chromophore design to classical Monte Carlo and molecular dynamics simulations for understanding ordering/packing and interactions with surfaces and electrodynamics calculations for understanding interactions with light in a device-relevant environment. This seminar will discuss the process of developing OEO materials through multiple levels of computational models, as well as lessons learned in translating this knowledge to commercial products.



Integrated BiCMOS/POH high-speed transmitter fabricated by collaborators at ETH-Zurich (Koch et al. 2020)

References:
U. Koch, et al., A monolithic bipolar CMOS electronic–plasmonic high-speed transmitter. *Nature Electronics* **2020**. doi:10.1038/s41928-020-0417-9
H. Xu, et al., Bis(4-dialkylaminophenyl)heteroarylamino donor chromophores exhibiting exceptional hyperpolarizabilities. *Journal of Materials Chemistry C* **2021**. doi:10.1039/d0tc05700b