

Risko Research Group

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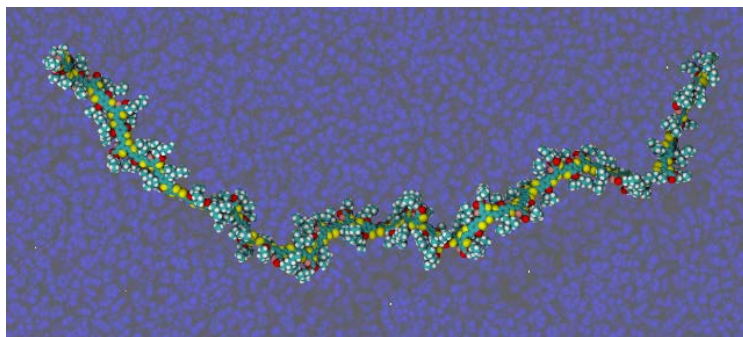
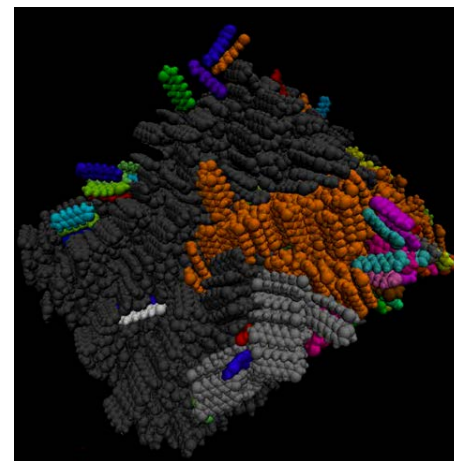


in silico Synthetic Materials Chemistry

Research in the Risko group is inspired by the complexities of synthetic materials.

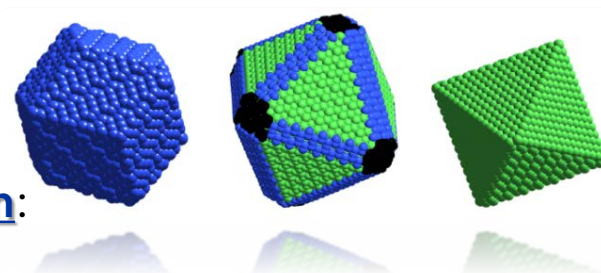
With emphasis in the areas of carbon electronics, power generation and storage, and catalysis, we bridge

- ✓ quantum chemistry
- ✓ classical molecular dynamics
- ✓ condensed-matter physics
- ✓ materials science
- ✓ polymer science
- ✓ data analytics
- ✓ computer science



to unravel chemical and physical phenomena at all stages of the materials pipeline.

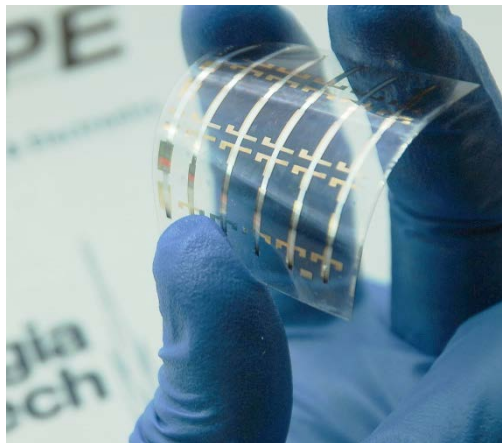
Ultimately, our aim is *in silico* materials design: materials invented on the computer!





Plastic (carbon) electronics & energy storage

Organic Field-Effect Transistors (OFET)



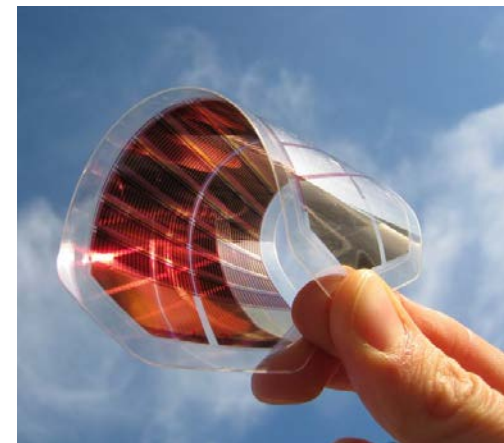
Georgia Institute of Technology

Organic Light-Emitting Diodes (OLED)

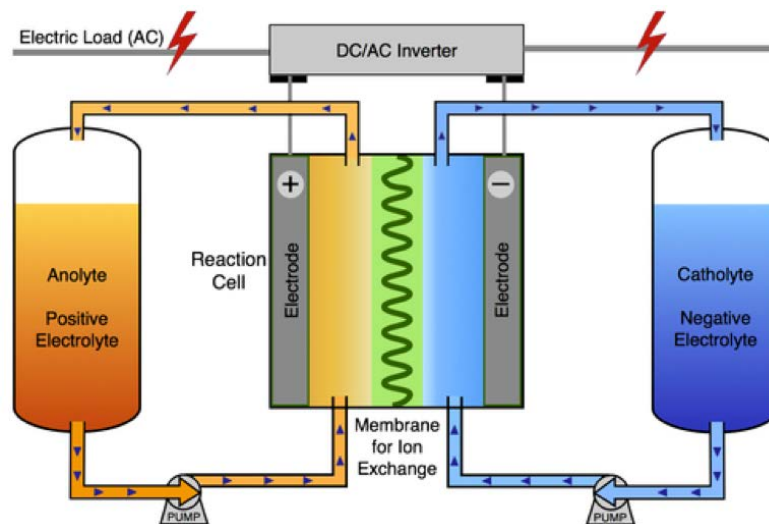
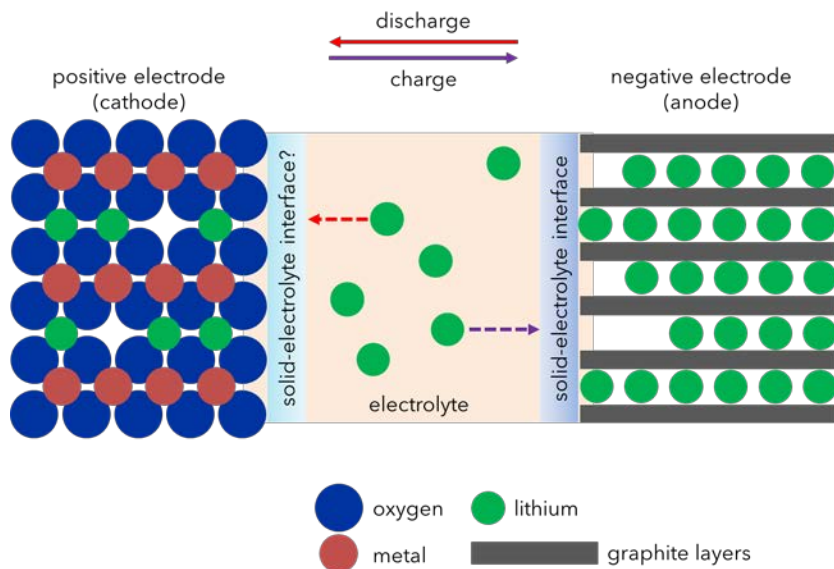


General Electric

Organic Photovoltaics (OPV)

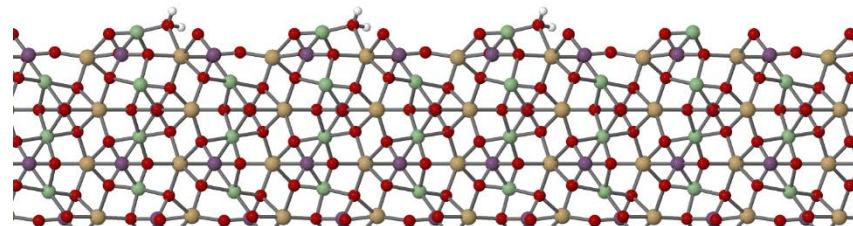
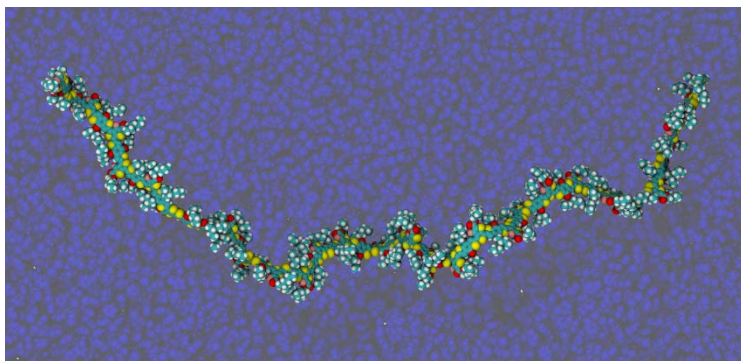


Fraunhofer Institute for Solar Energy Systems (ISE)

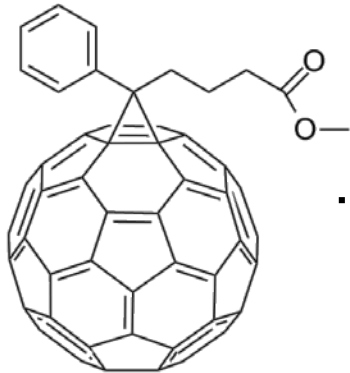
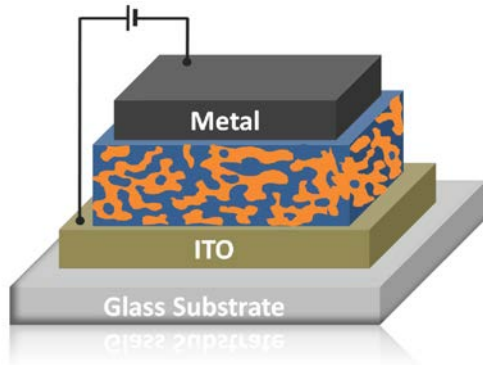


The problems that we are interested in solving range across many length and time scales. This requires that our theoretical materials chemistry approaches be truly multiscale. We therefore make use of:

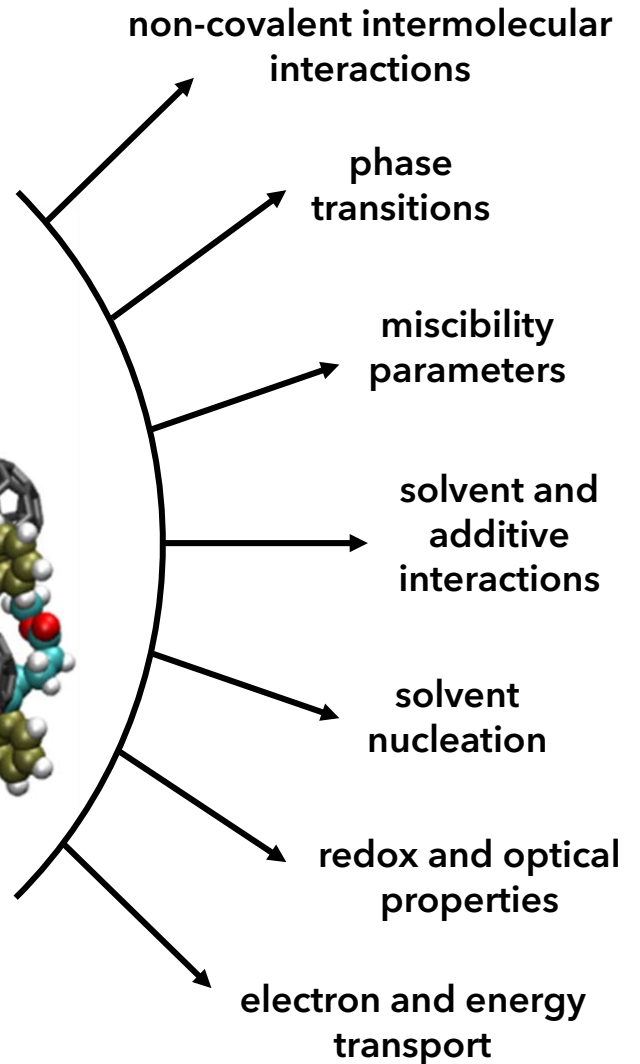
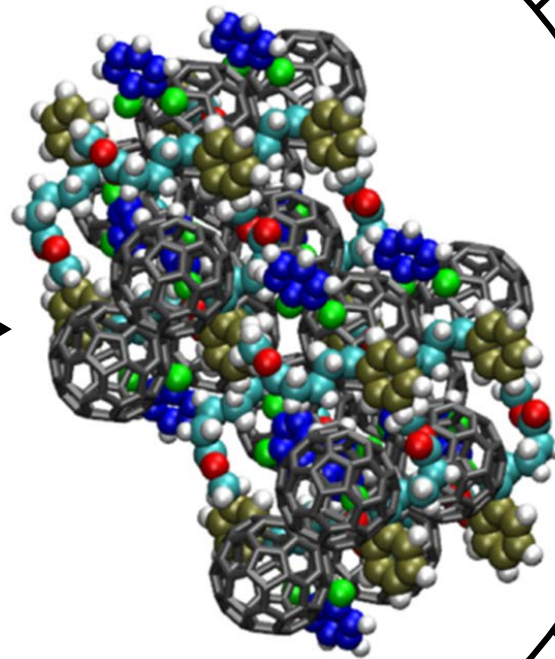
- electronic-structure theories:
 - density functional theory (DFT)
 - wavefunction methods, including high-level electron-correlation and perturbation methods
- atomistic and coarse-grained molecular dynamics simulations
- condensed-matter physics
- thermodynamic and kinetic models



Harnessing solar energy with OPVs



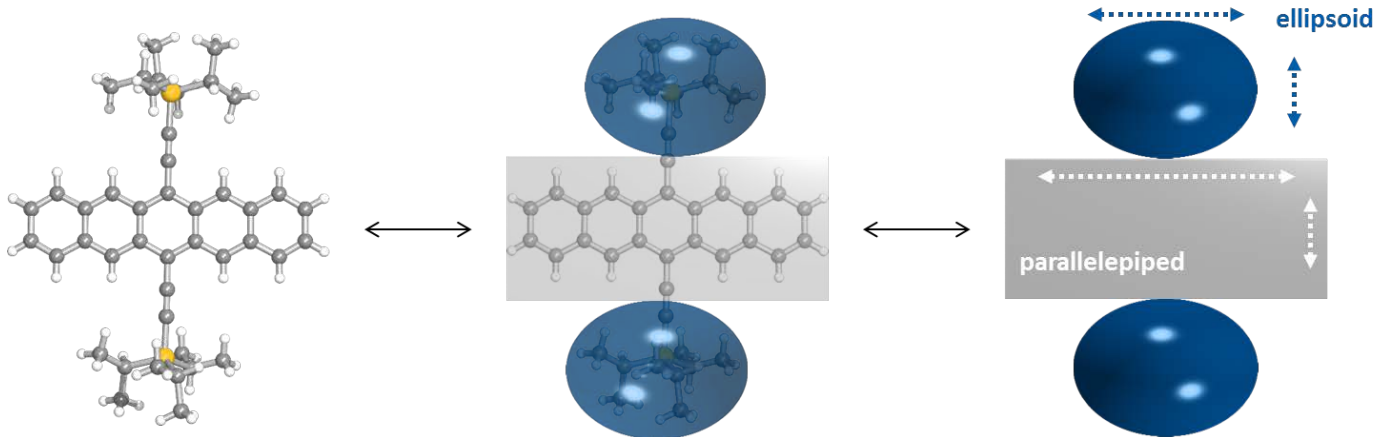
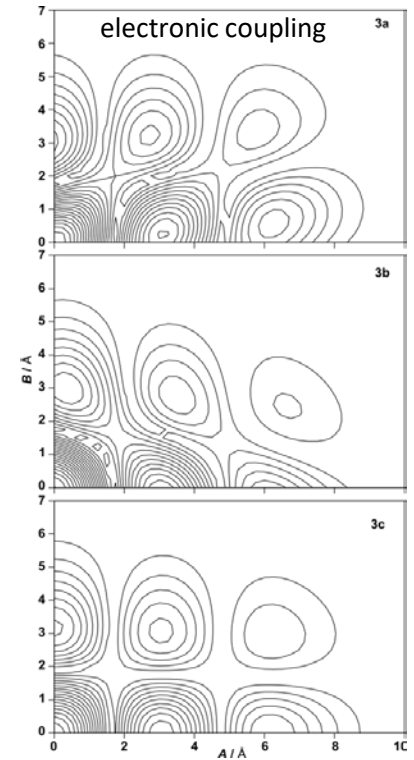
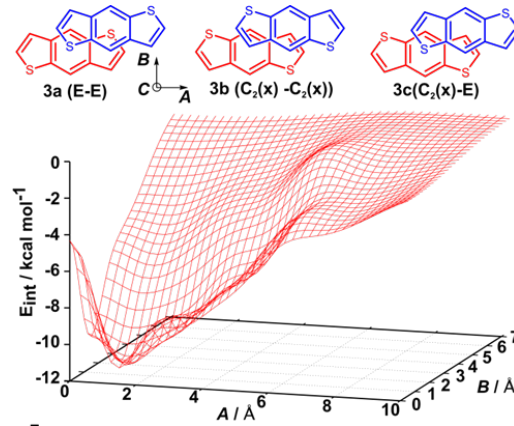
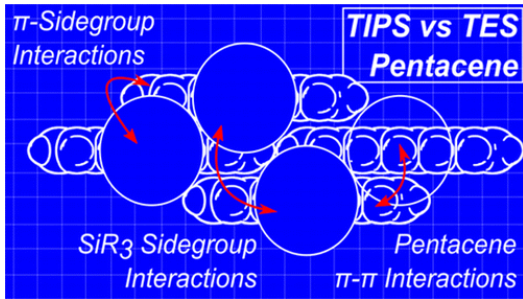
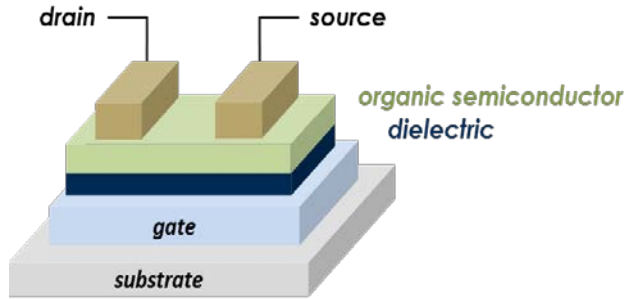
chemical substitution →

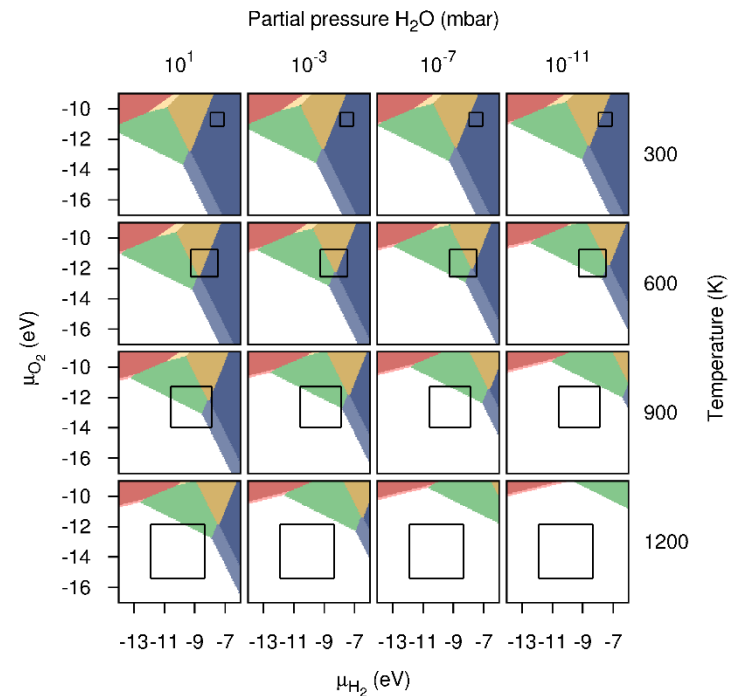
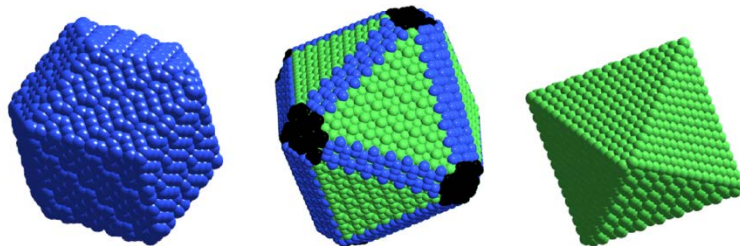
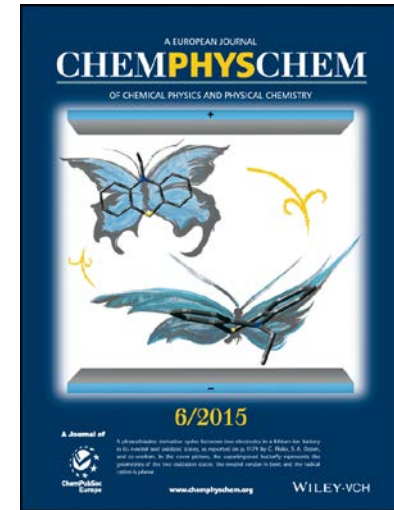
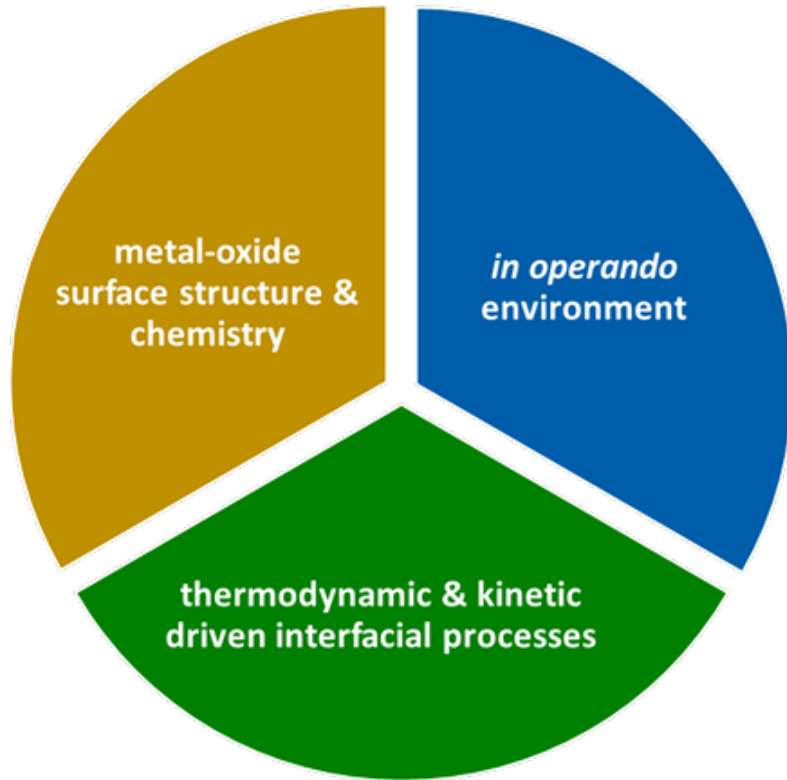


chemical composition & structure

molecular packing

material characteristics and morphology







- Where do we apply for and obtain funding?
 - National Science Foundation
 - Department of Energy
 - Office of Naval Research

- Where do we publish?
 - Journal of the American Chemical Society; Advanced (Functional) Materials; Chemistry of Materials; Journal of Materials Chemistry; ACS Applied Materials and Interfaces; Journal of Physical Chemistry...

- Where do we go for conferences?
 - American Chemical Society; Materials Research Society
 - Gordon Research Conference
 - Functional π Materials; International Conference on Synthetic Metals