

Risko Research Group

theoretical materials chemistry in the Bluegrass

Chad Risko

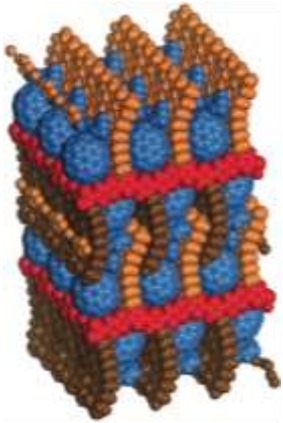
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develop and implement theoretical materials chemistry approaches
to uncover critical relationships among:

molecular / polymer / metal-oxide composition & solid-state structure



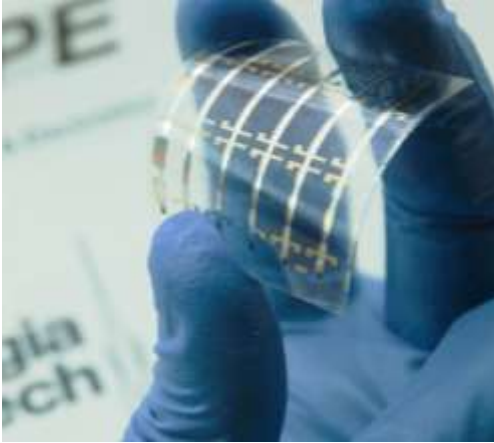
electronic, redox, and optical properties



novel materials of interest for
energy conversion and storage applications &
new generations of electronic and optoelectronic devices

Plastic (carbon) electronics

Organic Field-Effect Transistors (OFET)



Center for Organic Photonics and Electronics
(COPE),
Georgia Institute of Technology

Organic Light-Emitting Diodes (OLED)



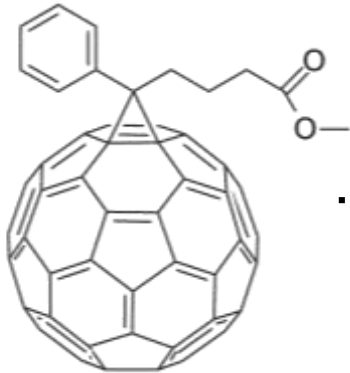
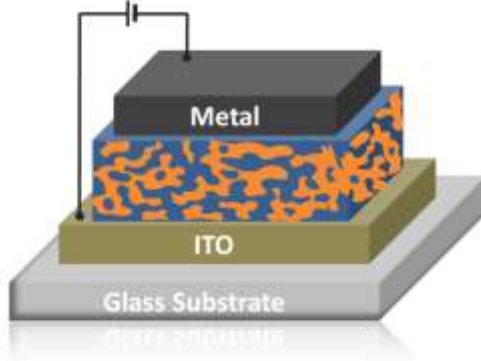
General Electric

Organic Photovoltaics (OPV)

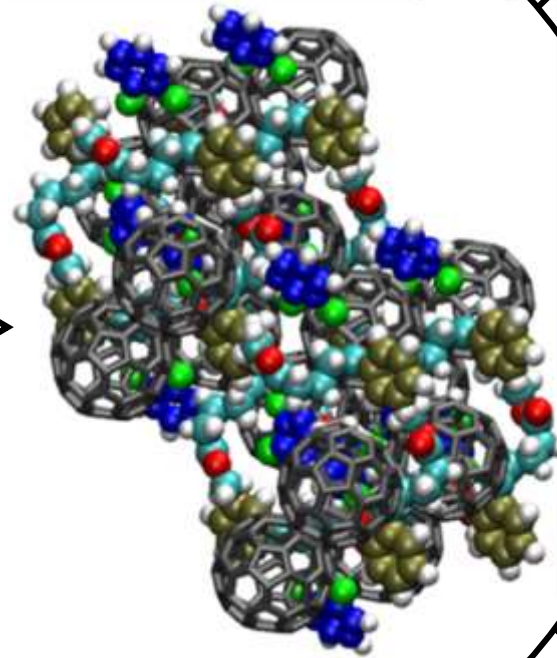


Center for Materials Research,
Freiburg (Baden-Wuerttemberg)
&
Fraunhofer
Institute for Solar Energy Systems (ISE)

Harnessing solar energy with OPVs



chemical substitution →



non-covalent intermolecular interactions

phase transitions

miscibility parameters

solvent and additive interactions

solvent nucleation

redox and optical properties

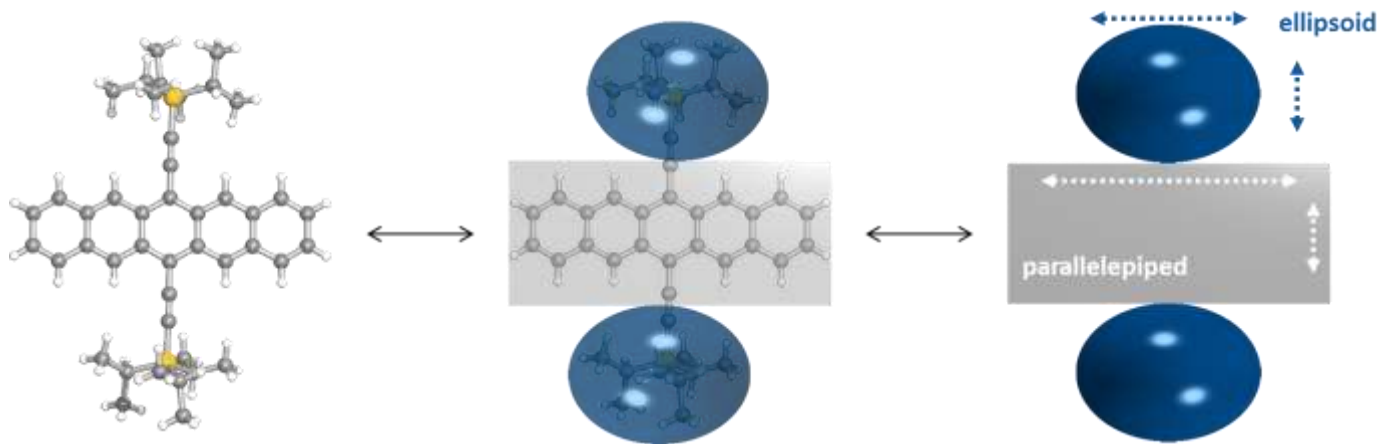
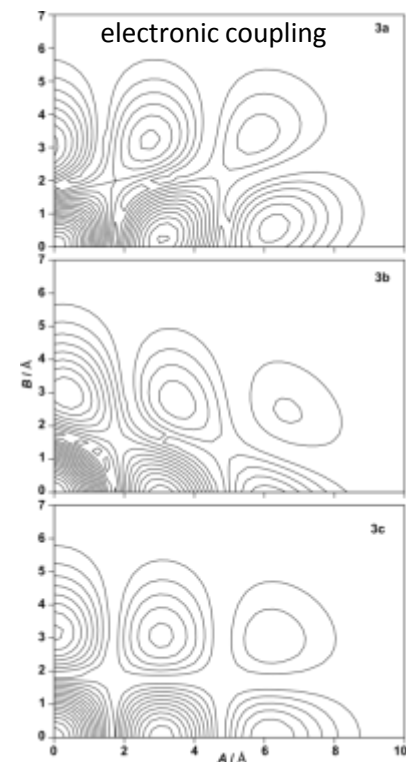
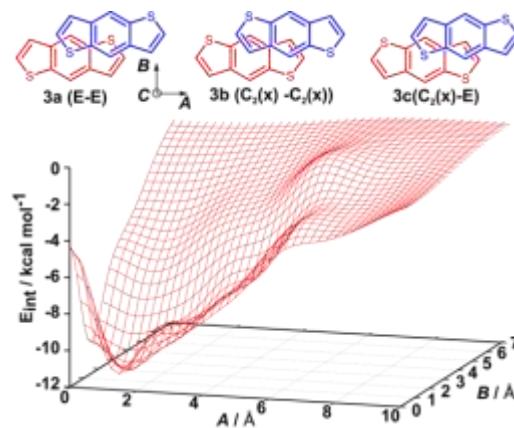
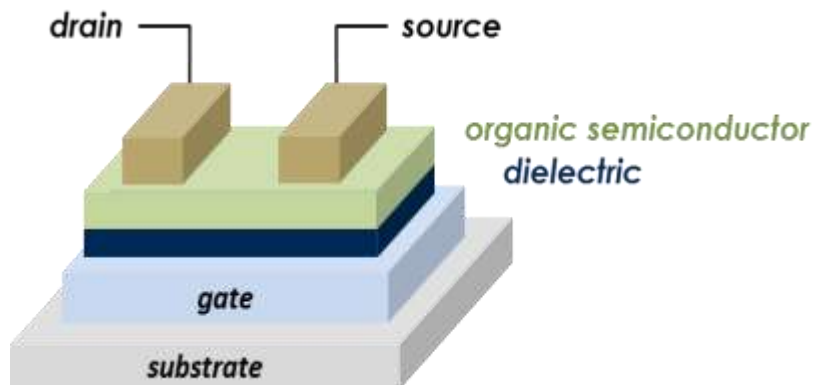
electron and energy transport

chemical composition & structure

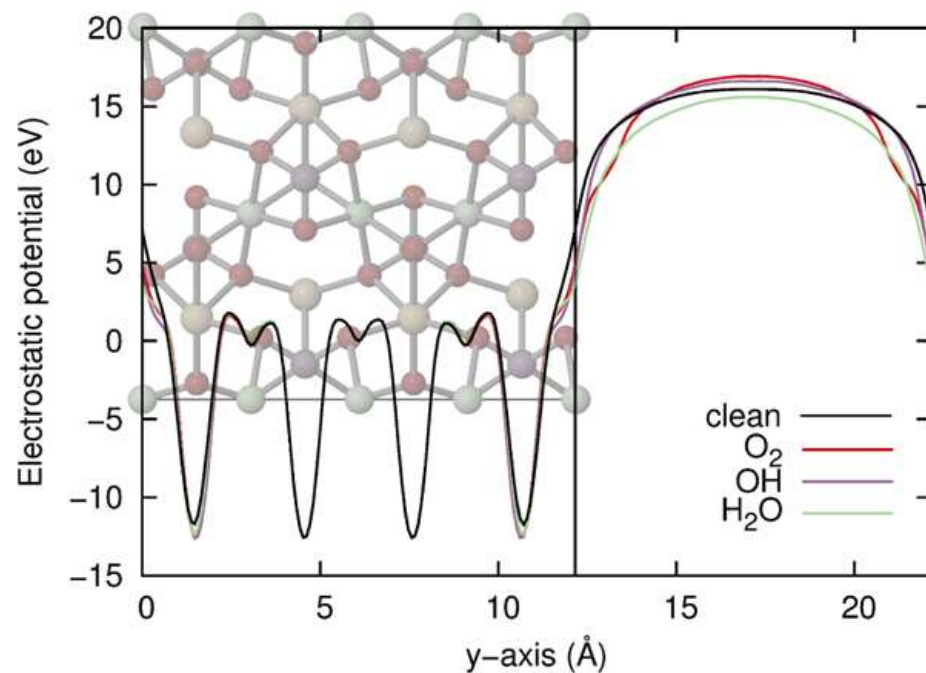
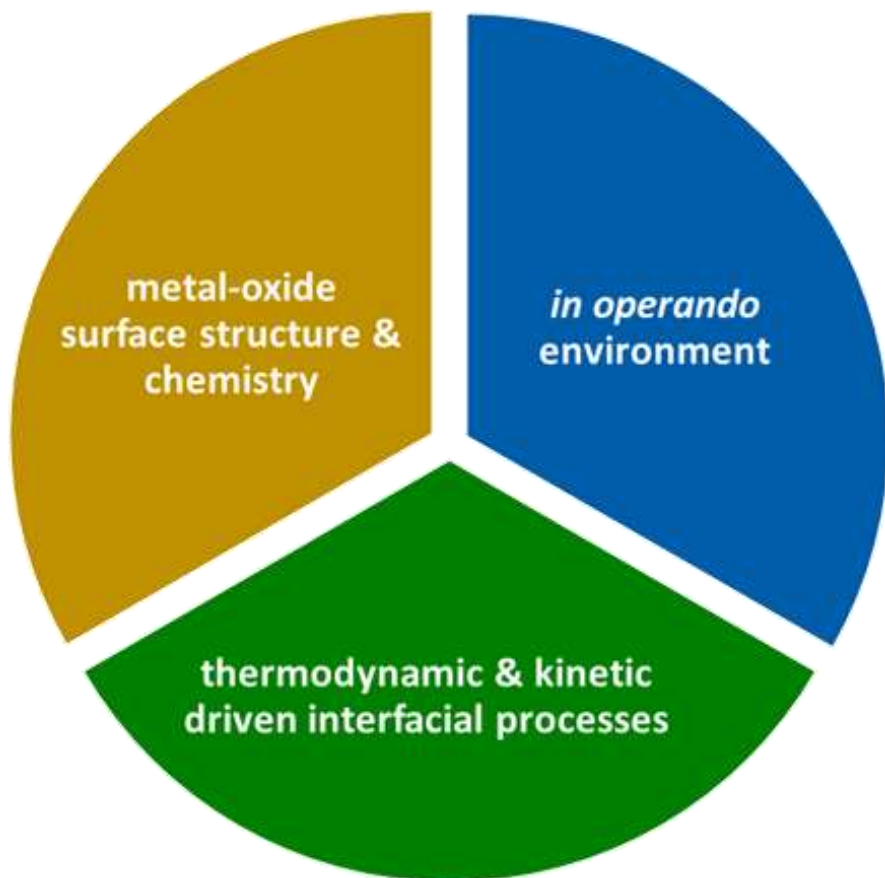
molecular packing

material characteristics and morphology

in silico Materials Design for OFET



Computational electrochemistry

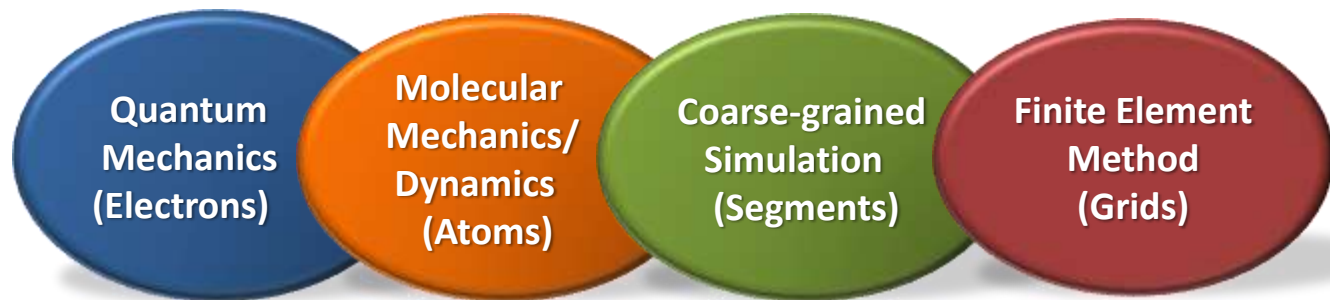
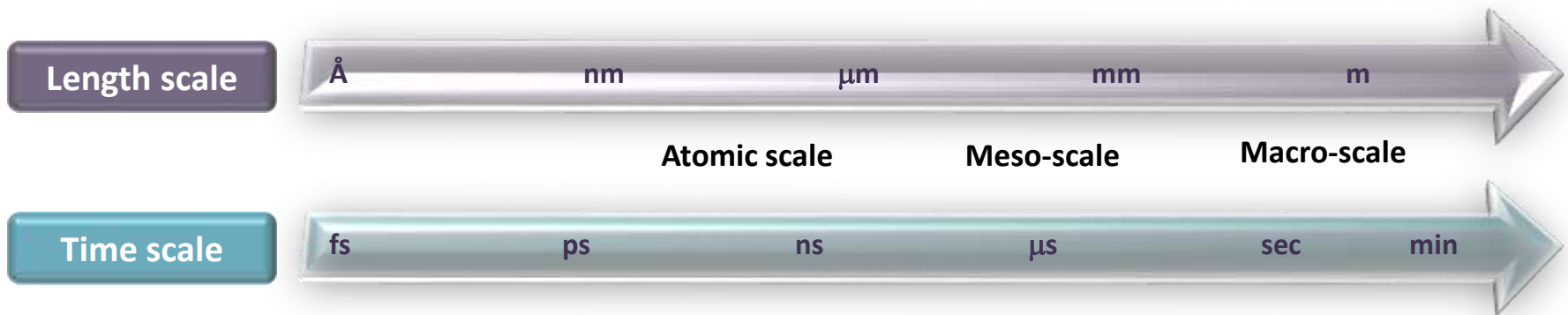


- Where do we apply for funding?
 - National Science Foundation
 - Department of Energy
 - Office of Naval Research

- 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

Multi-scale computational modeling



$$H\psi = E\psi$$

$$F = ma$$

Geometric and electronic structure

Conformational search

Morphology

Macroscopic processing

Optical and electronic properties

Crystalline/amorphous structure

Dynamic evolution of a large system
Structural analysis

Chemical reactions