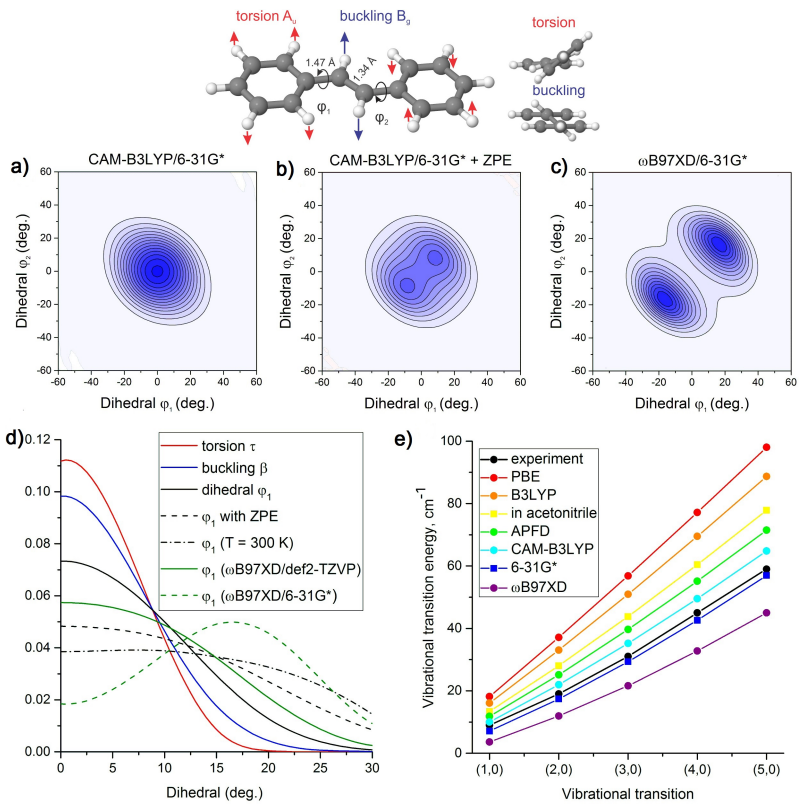
Structural studies: slide 1 of 2

(first-principles at DFT-D accuracy, up to 1000 atoms in simulation cell)

Molecules

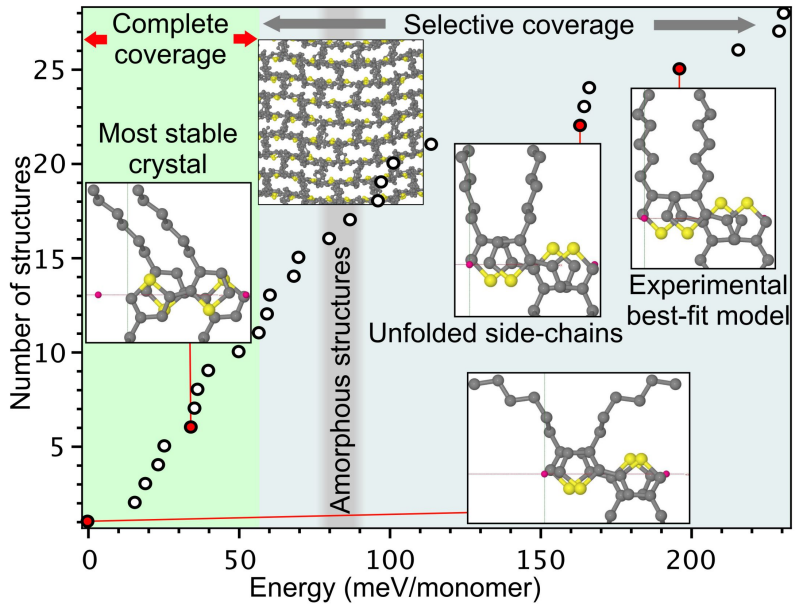
Is stilbene (and PPV) planar or not?



J Phys Chem Lett 10, 3232 (2019)

Structure prediction for polymers

What is the local structure of P3HT?



J Phys Chem C 122, 9141 (2018)

Ongoing efforts:

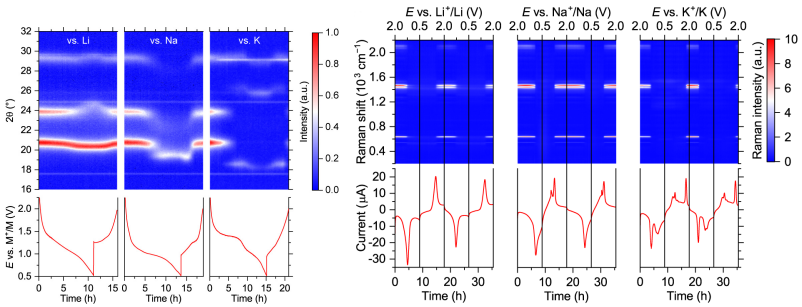
cmsos.github.io/escp

Structural studies: slide 2 of 2

(first-principles at DFT-D accuracy, up to 1000 atoms in simulation cell)

Predict structural changes

How alkaline ions intercalate into?

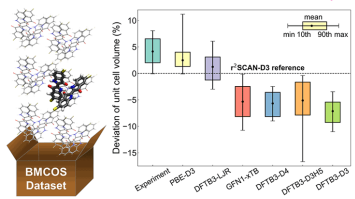


Chem Sci 13, 8161 (2022)

Ongoing efforts: impurities creating electronic traps

Computer-aided design of materials

- Structure refinement
  - from experiment
  - from structural models
  - from force field models
- Benchmarking methods
  cmsos.github.io/bmcos



JCTC 19, 8481 (2023) – 67 crystals

- Exploring novel architectures
  - frameworks
  - 2D/3D polymers
  - wiremesh Chem Mater 33, 966 (2021)
  - nonplanar π-systems
  - interdigitated herringbone

Electronic properties of materials: slide 1 of 2

(scalable approaches $\Longrightarrow$ multiscale modeling, DFT-parametrized effective Hamiltonian)

Electronic/vibrational spectroscopy

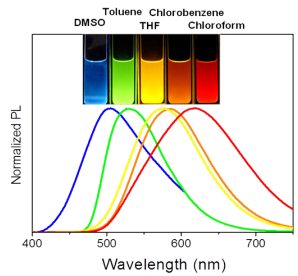
Commonly used to probe local structural and electronic properties

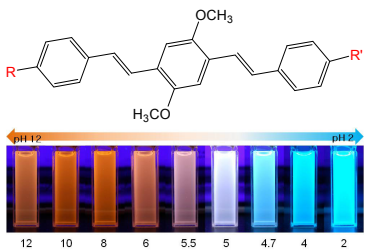
- Derive structural information

  J Phys Chem Lett 10, 3232 (2019) – stilbene

  Chem Sci 13, 8161 (2022) – charging
- Screen out inaccurate methods

  Chem Sci 13, 8161 (2022) – by bandgap
- Understand spectral changes





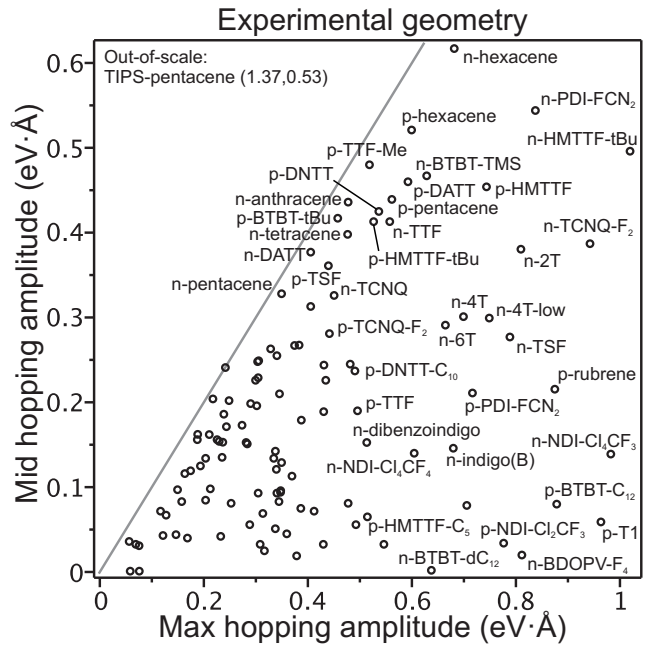
ACS Appl Mater Interfaces 5, 4685 (2013)

Chem Sci 6, 789 (2015)

Chem Phys 481, 133 (2016)

Charge carrier transport

How to quickly estimate mobility?



(ongoing project)

What is the origin of nonmonotonic temperature dependence of luminescence kinetics?

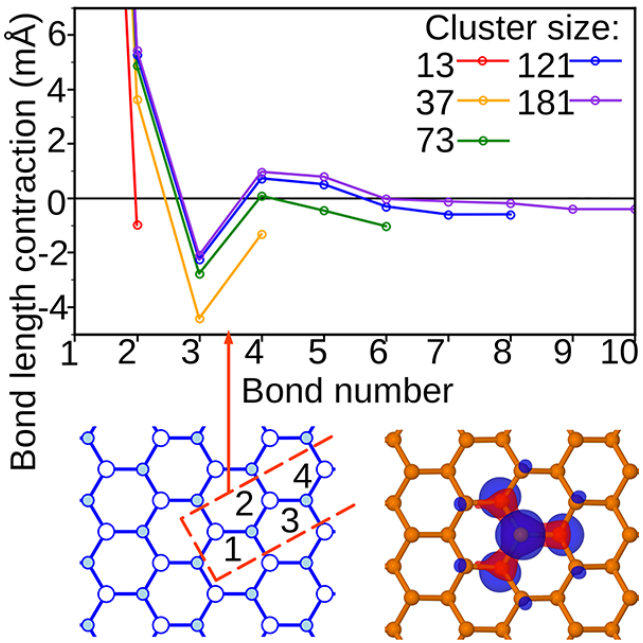
Low Temperature Physics 28, 706 (2002)

Electronic properties of materials: slide 2 of 2

(scalable approaches $\Longrightarrow$ multiscale modeling, DFT-parametrized effective Hamiltonian)

Polarons, electron-phonon dynamics

Do small polarons exist in nonpolar inorganic semiconductors?



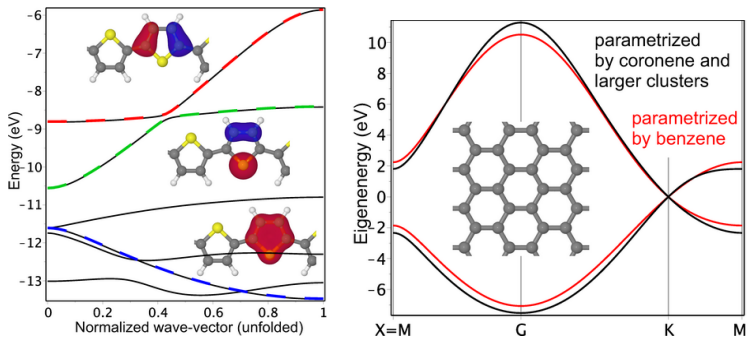
J Phys Chem Lett 12, 4674 (2021)

How to model electron-phonon dynamics faster than NAMD but more accurately than KMC?

Electronic Coarse-Graining

Method+code to model electronic structure of complex semiconductors

zhugayevych.me/research/ECG



J Chem Phys 159, 024107 (2023)

Ongoing efforts:

- cmsos.github.io/escp
- cmsos.github.io/tbm (library of electronic prototypes)
- excited states
- add vibronic couplings