OLED tools

… the atomistic part of our multiscale toolchain

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Two step process:

1. Deposition workflow

2. Properties workflow

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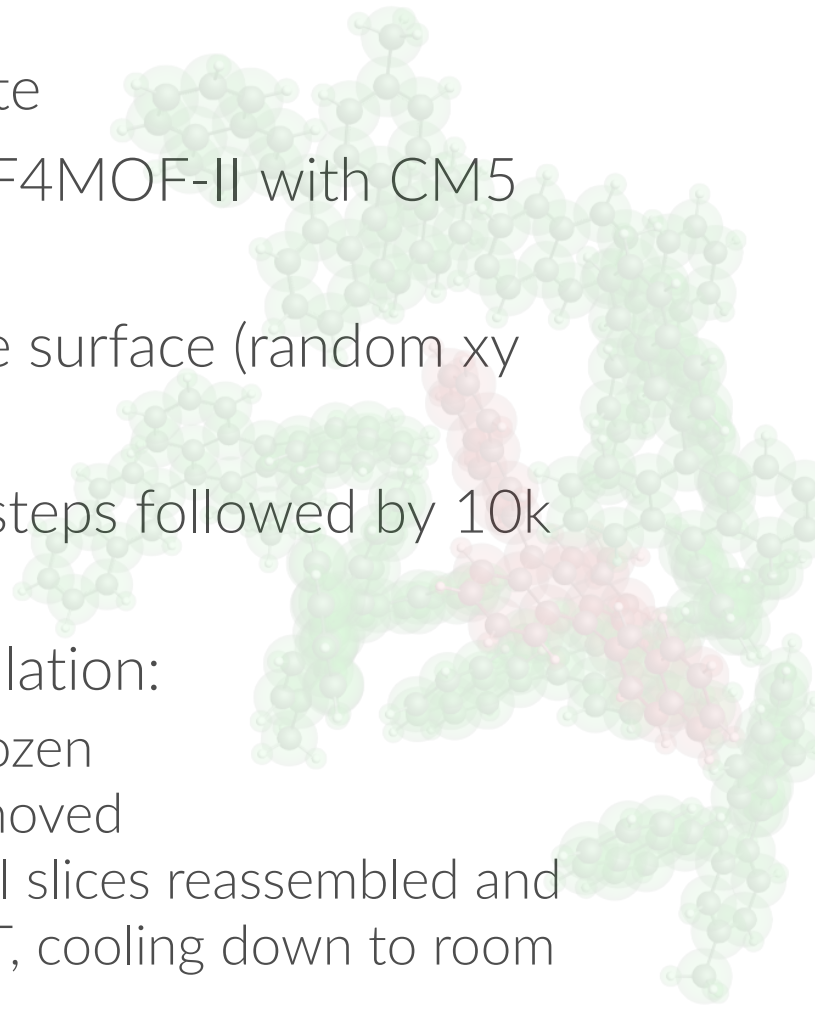
Deposition workflow

- Graphene sheet as starting substrate
- Molecules parameterized using UFF4MOF-II with CM5 charges
- Each molecule inserted 1 nm above surface (random xy position)
- After each insertion, 10k 1-fs MD steps followed by 10k fbMC steps to let molecule settle
- Periodic trimming to speed up simulation:
  - Molecules deep below surface frozen
  - Molecules below frozen layer removed
  - After reaching target thickness, all slices reassembled and whole box equilibrated under NpT, cooling down to room temperature



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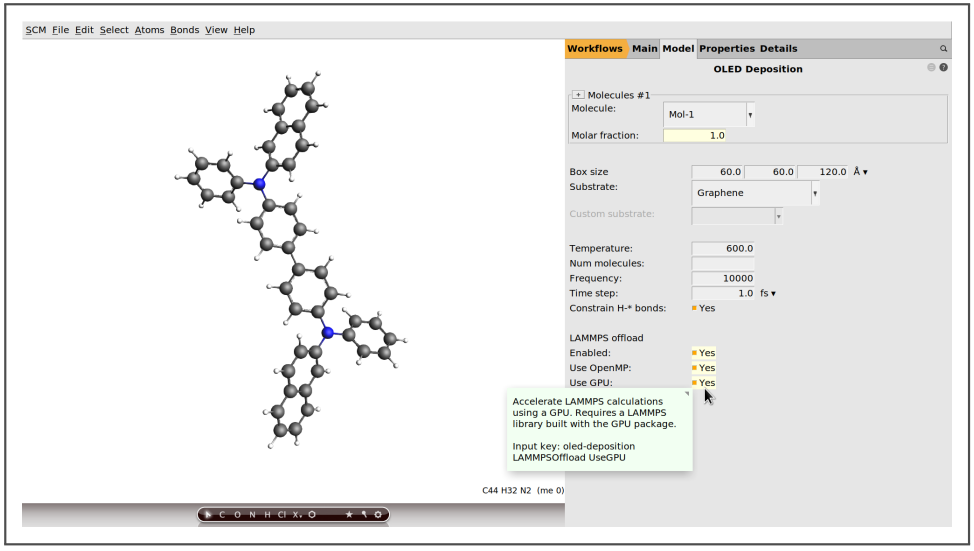
Deposition workflow

New in AMS2023: LAMMPS/GPU offloading

- Speedup of factor ≈ 5
- 2 weeks $\Rightarrow$ 3 days (standard box of 6x6x6 nm with approx. 500 molecules)



- requires user to compile LAMMPS
  - enabling GPU and OPENMP packages highly recommended
  - can work with CUDA or OpenCL, depending on how you configure LAMMPS
- communication between AMS driver and LAMMPS via AMSPipe protocol:

  `https://www.scm.com/doc/AMS/Pipe_protocol.html`

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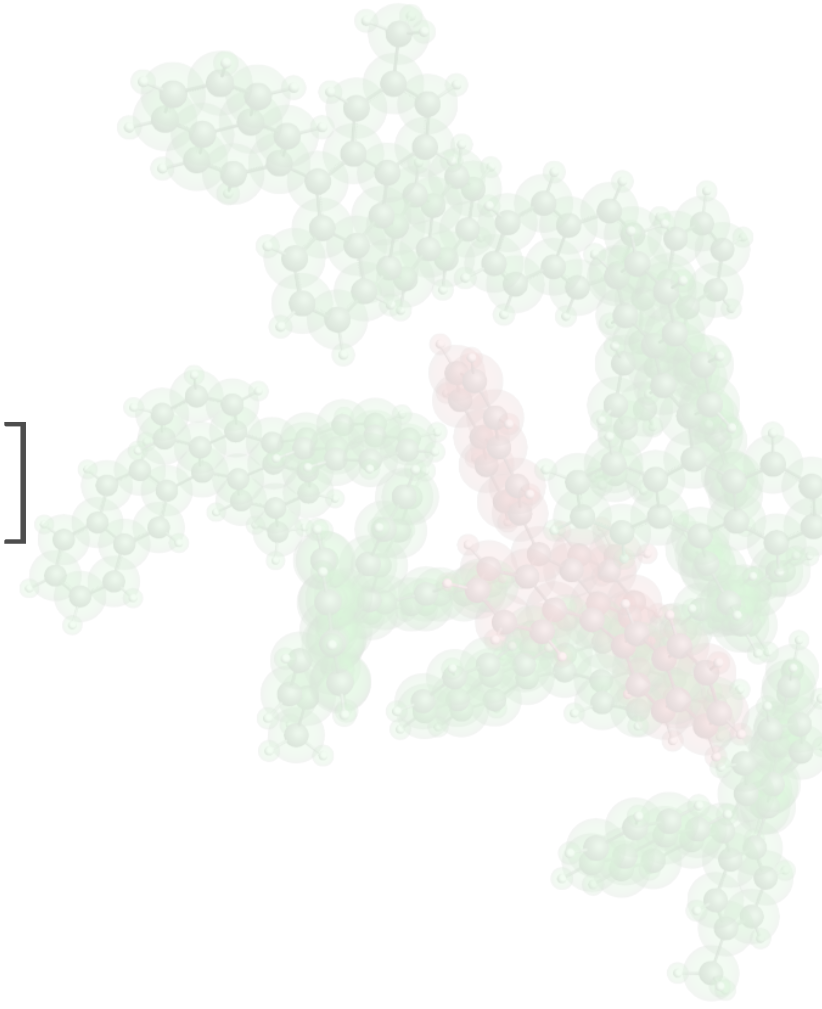
Deposition workflow

[Demo]



Deposition workflow

[Video]

downloads.scm.com/distr/OLEDTools_videos/deposition_mCP_1080p.mp4

Deposition workflow

Validation against thin-film densities

Material	$\rho_{calc.}$	$\rho_{exp.}$ [1]
BCP	1.148	1.12 ± 0.01
CBP	1.184	1.18 ± 0.01
α-NPB	1.114	1.19 ± 0.01
α-MADN	1.142	...
mer-Alq3	1.272	1.31 ± 0.01

Densities do not differ much between materials ...

[1] Review of Scientific Instruments 78, 034104 (2007); https://doi.org/10.1063/1.2712932

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Properties workflow

1. For each molecule in the box:
   - Calculate atomic charges with cheap DFT:
     LDA/DZP with MDC-D charge model
2. For each molecule in the box:
   - Determine environment:
     any molecule within 15 Å (atom-atom distance)
   - For $q \in \{-1, 0, +1\}$:
     - Optimize geometry of central molecule in frozen environment:
       GFN1-xTB in UFF4MOF-II with electrostatic embedding
     - DFT single point on the optimized geometry:
       PBE/TZ2P (all-electron) with DRF environment
     - If $q = 0$: TD-DFT (PBE0) calculation for excitation energies.
   - Calculate (approximately adiabatic) IP and EA from total energy differences.
3. Transfer integrals for all dimers within 4 Å (atom-atom) distance of each other.

All default settings. Some things can be tweaked by the user ...

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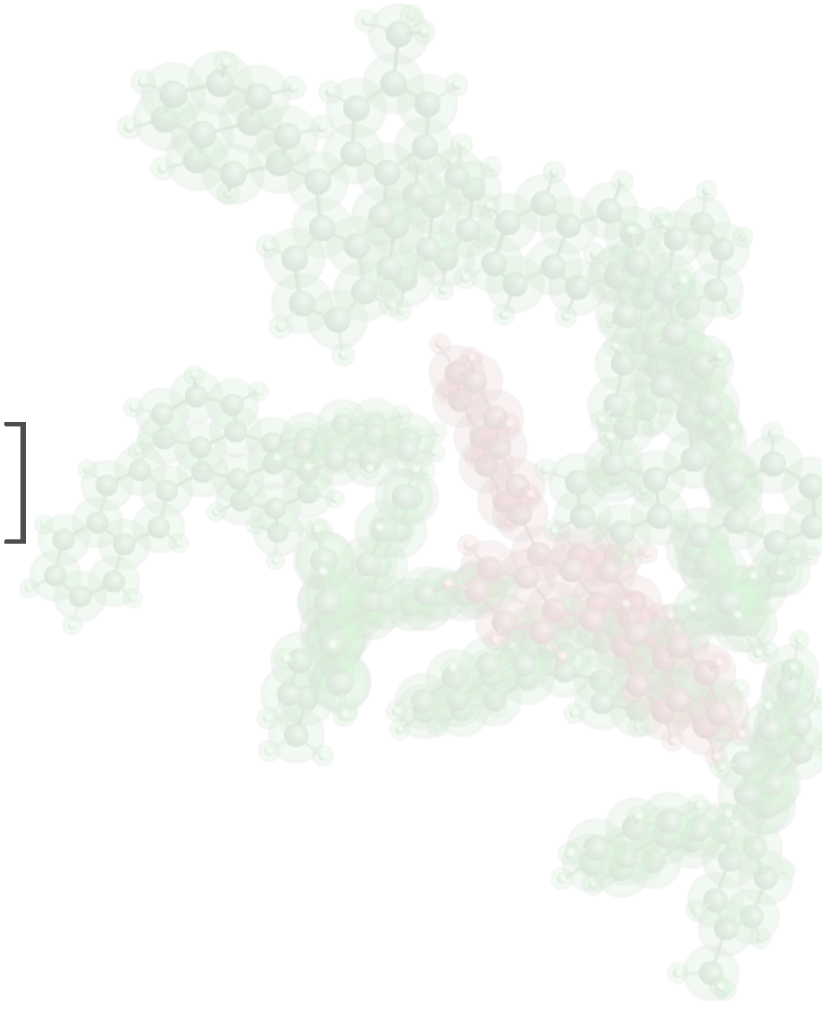
Properties workflow

[Video]

downloads.scm.com/distr/OLEDTools_videos/rotate_QMMM_mCP.mp4

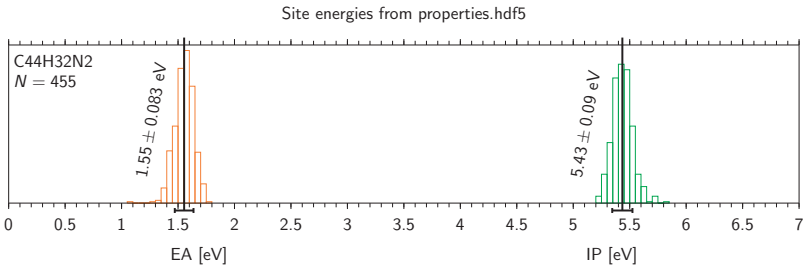
Properties workflow

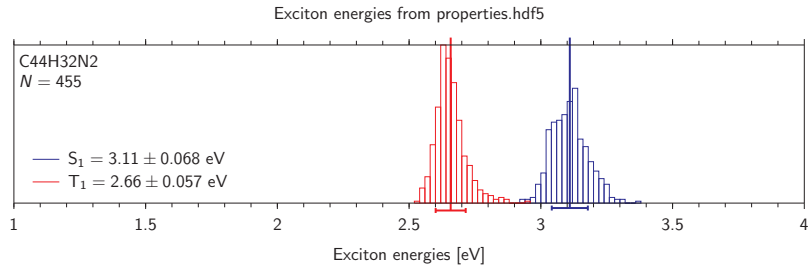
[Demo]

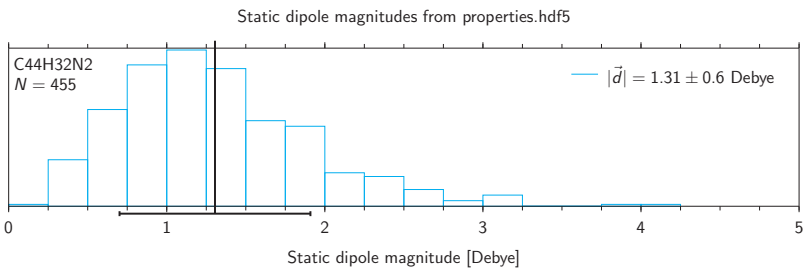


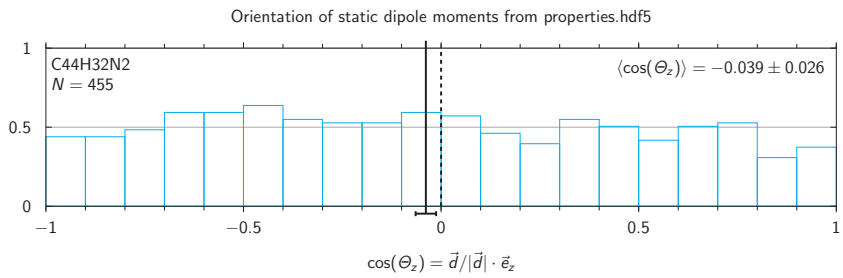
Properties workflow

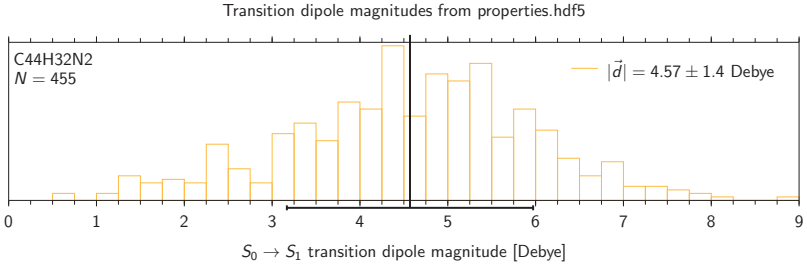
Results for α-NPB: site energies and dipole moments

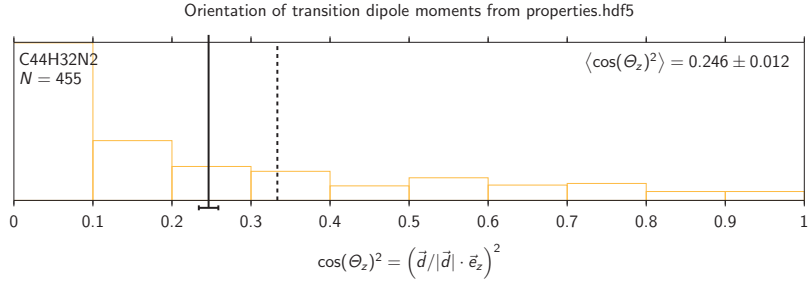






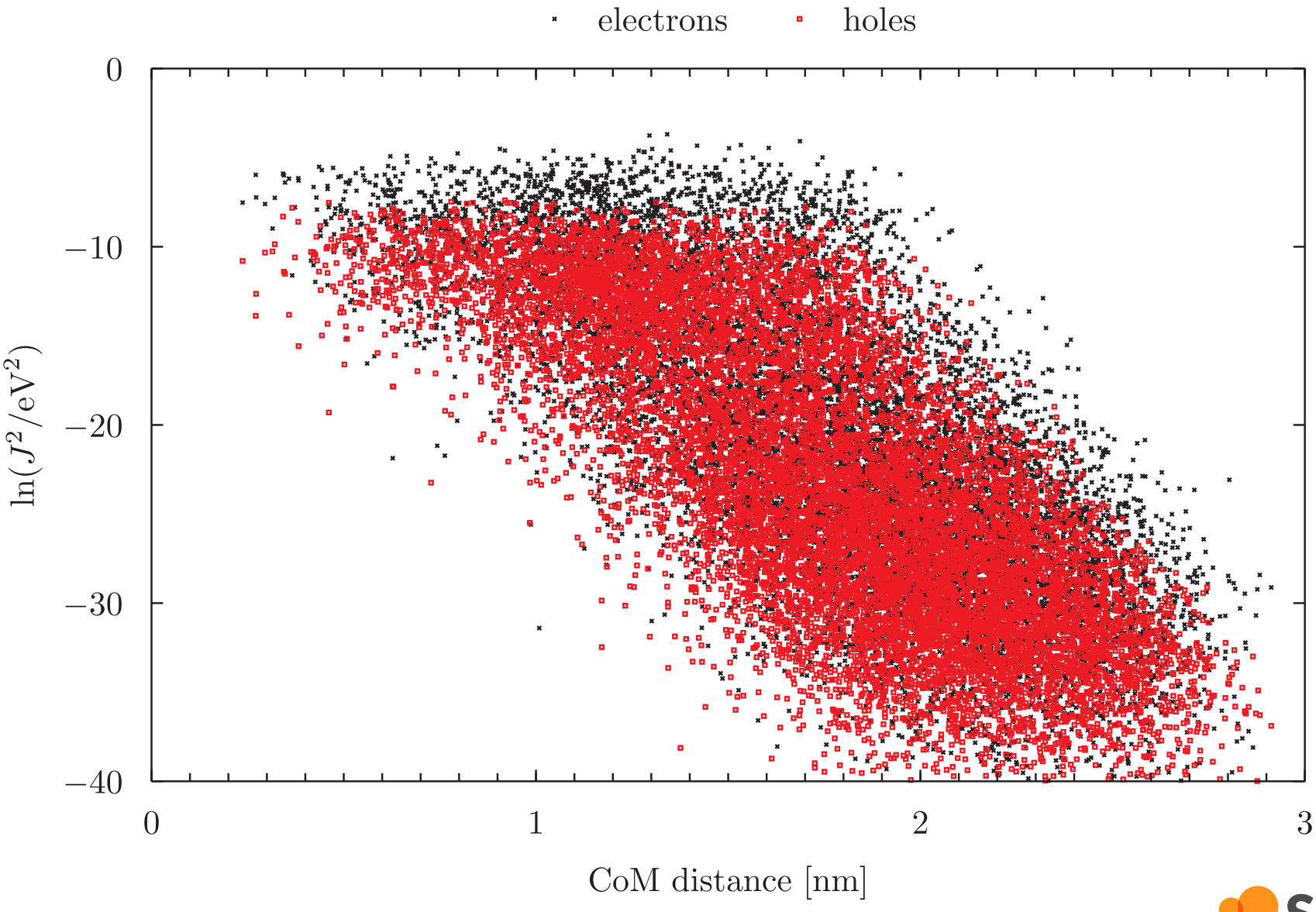






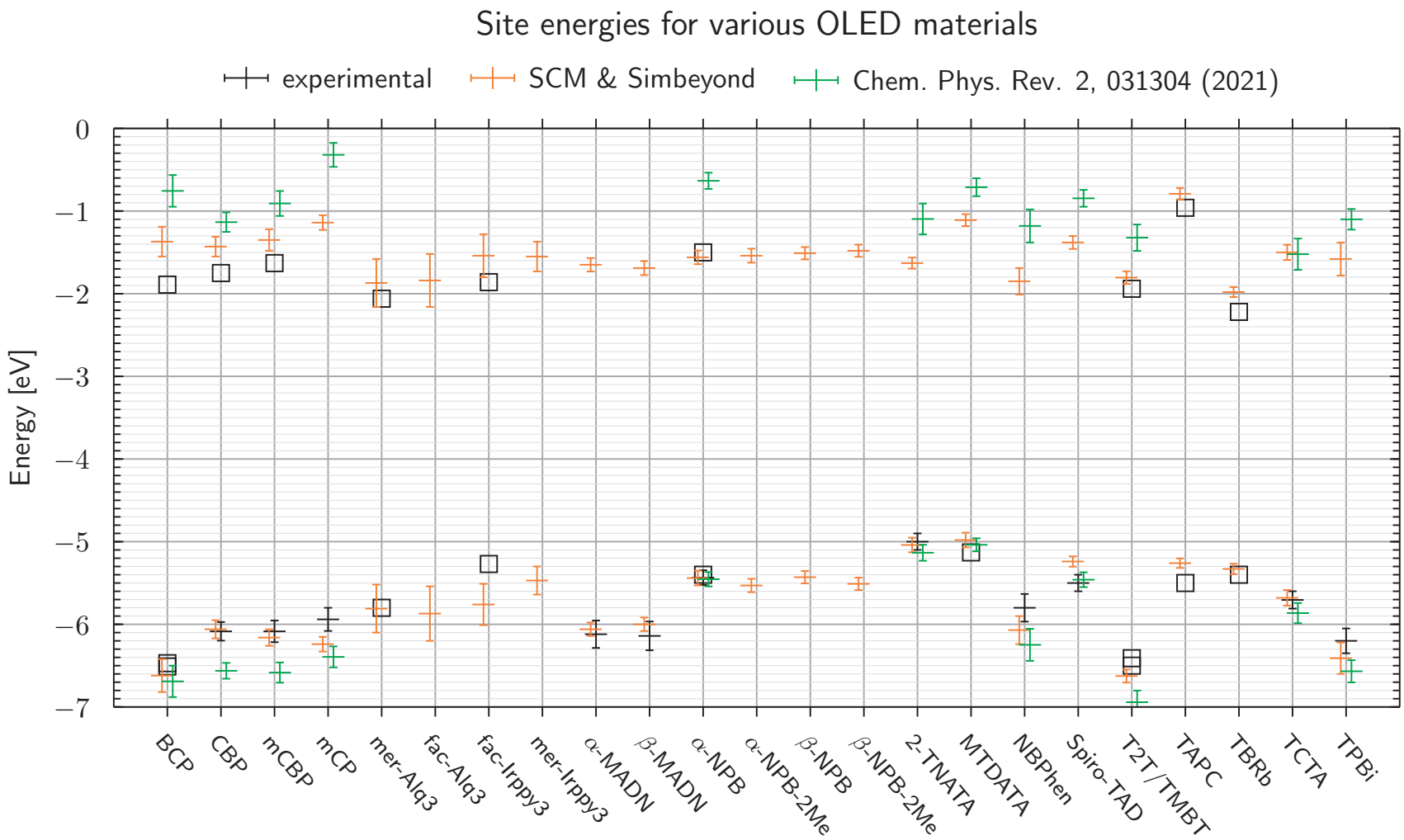
Properties workflow

Results for α-NPB: transfer integrals



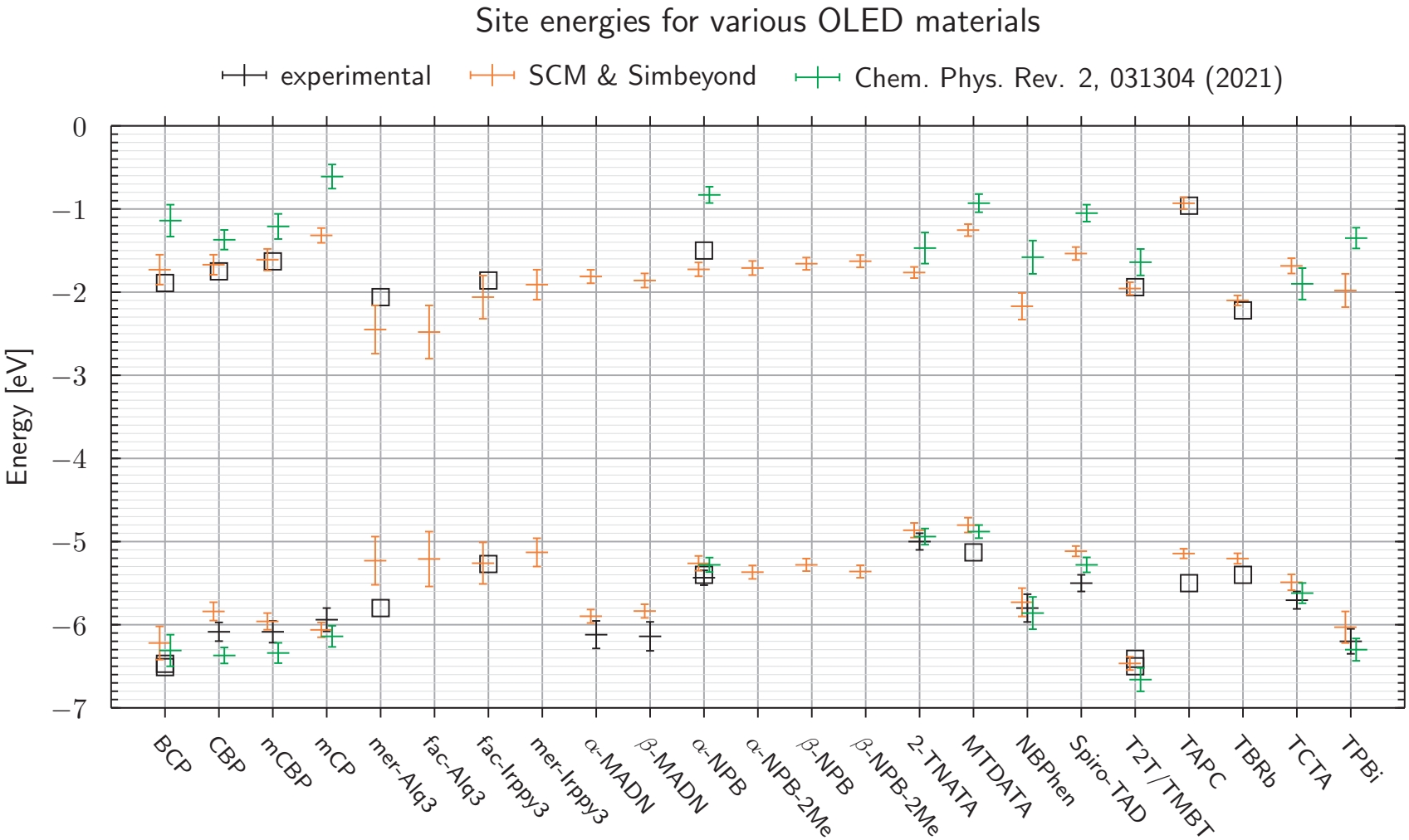
Properties workflow

Validation on IP/EA for standard materials [distribution means]



Properties workflow

Validation on IP/EA for standard materials [IP/EA $\pm 2\sigma$]



Plans for AMS2024

Further improvements for deposition workflow

1. whole-molecule moves in the force-bias Monte-Carlo part of the deposition:
   - increased mobility = better morphologies (?)
2. automated conformer handling for the deposited molecules:
   - currently we deposit a single conformer by default ..
   - ... whichever one the user puts into the input
   - no major conformational changes during MD in deposition
3. reduce protocol overhead in AMS $\leftrightarrow$ LAMMPS communication
   - currently there is an inefficient Python glue-layer inbetween
   - can be done directly Fortran $\leftrightarrow$ C++
   - expected speed-up of 3x $\Rightarrow$ deposition in ≈ 1 day
4. re-deposit all standard materials for OLED material DB 2024

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Plans for AMS2024

Further improvements for the properties workflow

1. GW/BSE for IP/EA and exciton energies
   - methods in AMS2023 already, but without support for DRF environment
   - equations have been derived by now, implementation in progress
2. more systematic validation of excition energies
3. more properties: (non-)radiative decay rates, intersystem crossing rates, …
4. increased range for transfer integrals
5. recalculate properties for all standard materials in OLED material DB 2024

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OLED workflows

[Tutorial]

www.scm.com/doc/Tutorials/WorkflowsAndAutomation/OLEDMaterials.html

[Manual]

www.scm.com/doc/AMS/Utilities/OLEDWorkflows.html

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