Hands-On Session Scripting

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Hands-On Exercise Scripting – Task

- Set of molecular structures… which of them have excitations < 4.0 eV?
  - TDDFT calculations are expensive → screening!
- Step 1
  - DFTB geometry optimizations & TDDFTB calculations
  - Find systems with excitation energy < 6.0 eV
    and oscillator strengths > 1E-4 Debye
- Step 2
  - ADF geometry optimization of structures found in step 1
- Step 3
  - TDDFT calculation
  - Determine systems with excitations < 4.0 eV (and > 1E-4 Debye)

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Hands-On Exercise Scripting – Files

- Download & unpack `TCCM_handsOn_Scripting.zip` from www.scm.com/collaborations/eu-projects/tccm-adf-tutorial
  - workflow.py ← script
  - molecules ← folder containing structures
- Run with `$(ADFBIN)/plams workflow.py`
  - Step 1, DFTB geometry optimization + TDDFTB calculation

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Hands-On Exercise Scripting – The Script

- Initial Section: Technical stuff (please do not change)
- Section “Step 1” (line 70)
  - Setup with auxiliary function `dftb_GO_plus_excitations`
  - Filtering excitations with `get_good_excitations`
  - Append potential candidates to list `promising_molecules`

Hands-On Exercise Scripting – Your Tasks

- Section “Step 2” (below line 86)
  - Create & run Job object `adf_GO_job` with settings function `adf_GO()`
  - `adf_GO_job.results.get_opt_molecule()`
  - Append molecule object to `optimized_molecules`
- Section “Step 3” (below line 100)
  - `adf_exci_job` with `adf_excitations(n_excitations=5)`
  - Run & filter good excitations below 4.0 eV (osc_str=1.0E-4)
  - Nicely print your results

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