**SYNERGISM BETWEEN THEORY AND EXPERIMENTS**

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**Examples:**
- **MD:** conformational sampling
  - Frames
  - Energy (kcal/mol)

- **DFT:** aromaticity index
  - Aromatic
  - Non-aromatic

- **TDDFT:** spectroscopy
  - Collaboration with C. Bolm (RWTH Aachen)
  - Org. Lett. 2019, 21, 4293

**Software:**
- HPRC: TERRA cluster
- DFT and TDDFT: Gaussian 16
- MD: Materials Studio
  - 28 cores, 24h
SYNERGISM BETWEEN THEORY AND EXPERIMENTS

DFT → Predict and assign $^{13}C\{^1H\}$ signals in platinum end-capped polyynes

HPRC: TERRA cluster
Gaussian 16 computational software
28 cores, 150 h
SYNERGISM BETWEEN THEORY AND EXPERIMENTS

DFT → Origin of Shielding and Deshielding Effects in NMR Spectra of Organic Conjugated Polyynes

HPRC: ADA cluster
DFT: Gaussian 16
20 cores, 6 h
SYNERGISM BETWEEN THEORY AND EXPERIMENTS

HPRC: ADA cluster
DFT: Gaussian 16
20 cores, 150+ h