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EURO

LITHUANIA

MOLECULAR SENSOR DESIGN USING HPC

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EuroCC@Greece HPC Training Series
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Science: BODIPY sensors and FLIM

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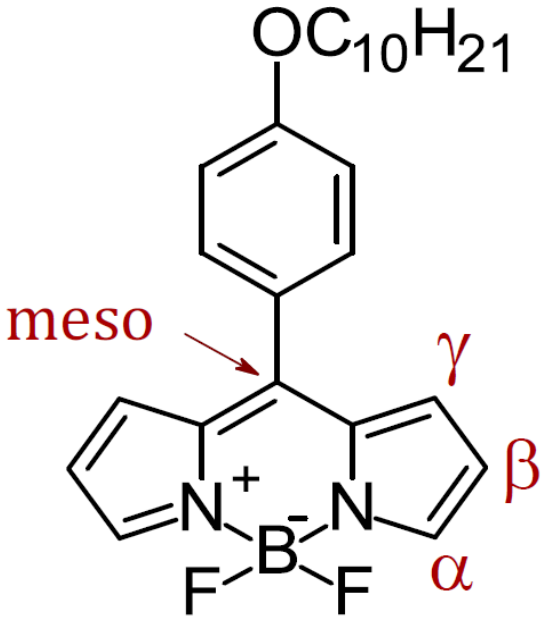
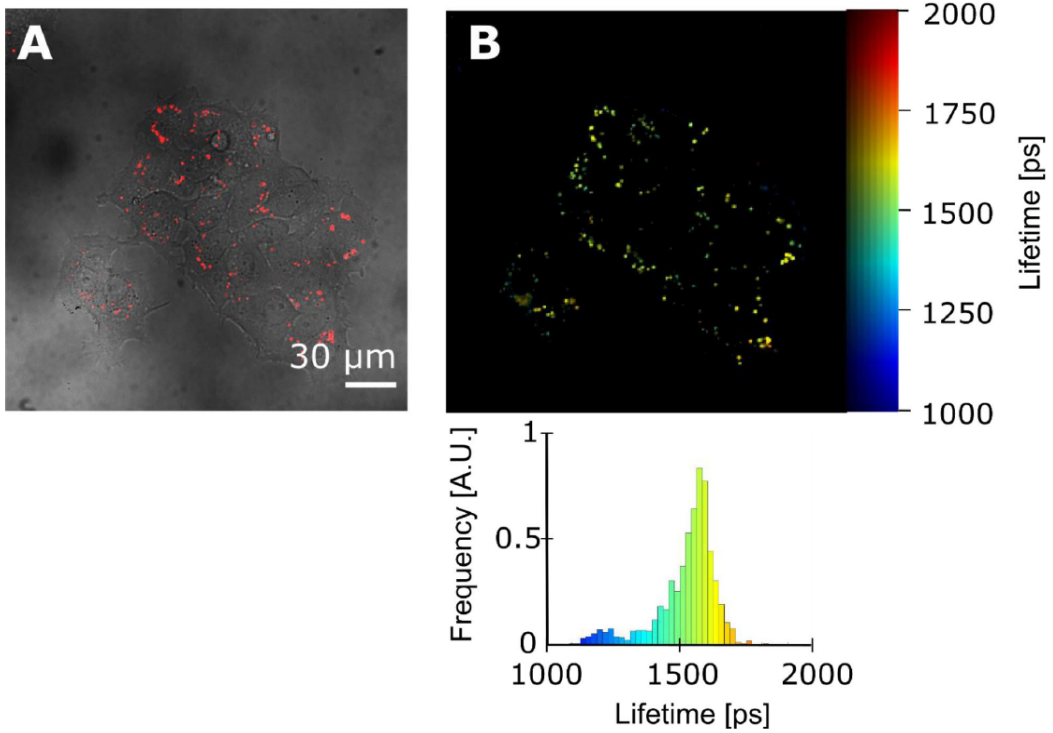


BODIPY-C_{10}



Maleckaitė *et al.*, *Chem Eur J.* **27** (2021)

PES model of viscosity sensitivity

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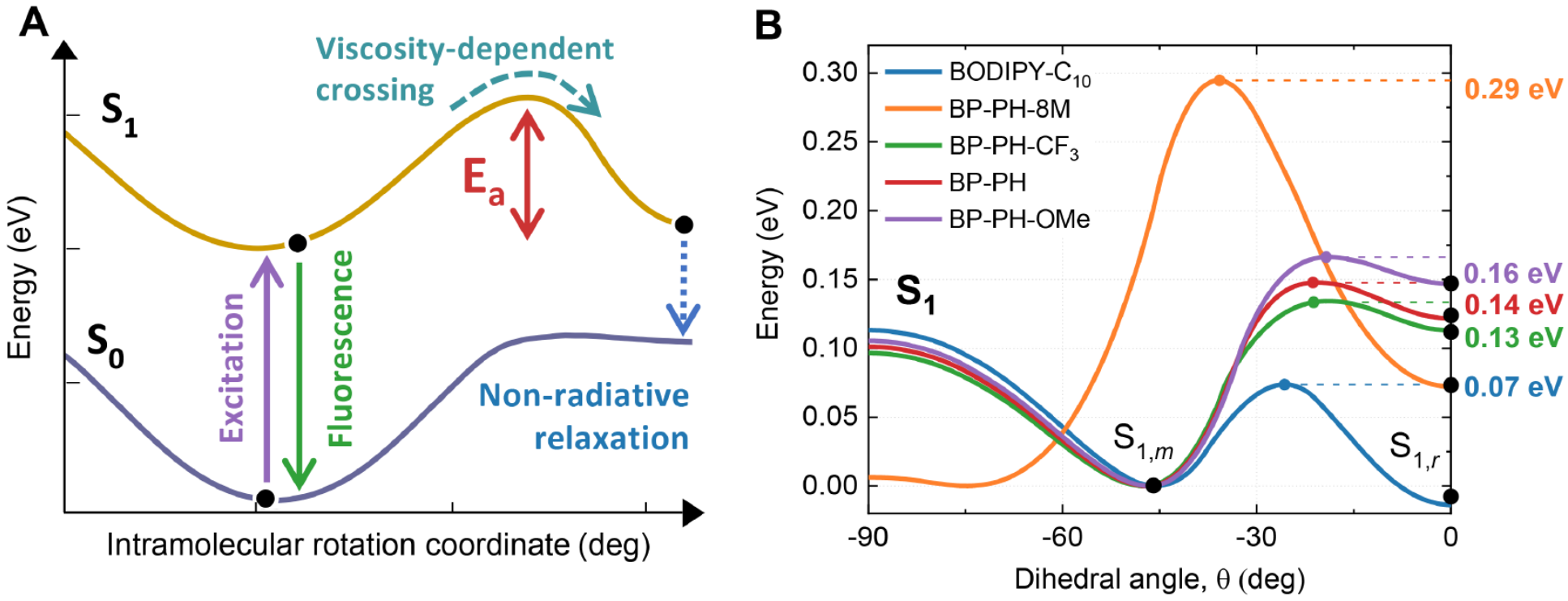

Maleckaitė *et al.*, *Molecules* **27** (2022)

Areas of improvement

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- Initial model is not suited for polar solvents
  - Local interactions with polarized solvent molecules

- Further interest in environment interactions/ dynamics
  - Viscosity vs. solvent granularity (Polita et al., 2020)
  - Selective staining of cell membranes (Polita et al., 2023)
  - BODIPY-formyl derivatives in methanol (*ongoing*)

Computing: methods

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- PES
  - (TD)DFT (M06-2x, cc-pVDZ) + CPCM (*Gaussian16*)
- Solvent shell
  - ONIOM (DFT / MM) (*Gaussian16*)
- Membrane
  - MM/MD with an adapted force-field (*GROMACS*)

Computing: local resources

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- VU HPC Saulėtekis *(Faculty of Physics location)*
  - 141 Bull Sequana X1000 nodes
    - ~0,3 PFlops (~20 TFlops / node)
  - 134 previous generations nodes
    - varying power/ availability

Computing cost – PES

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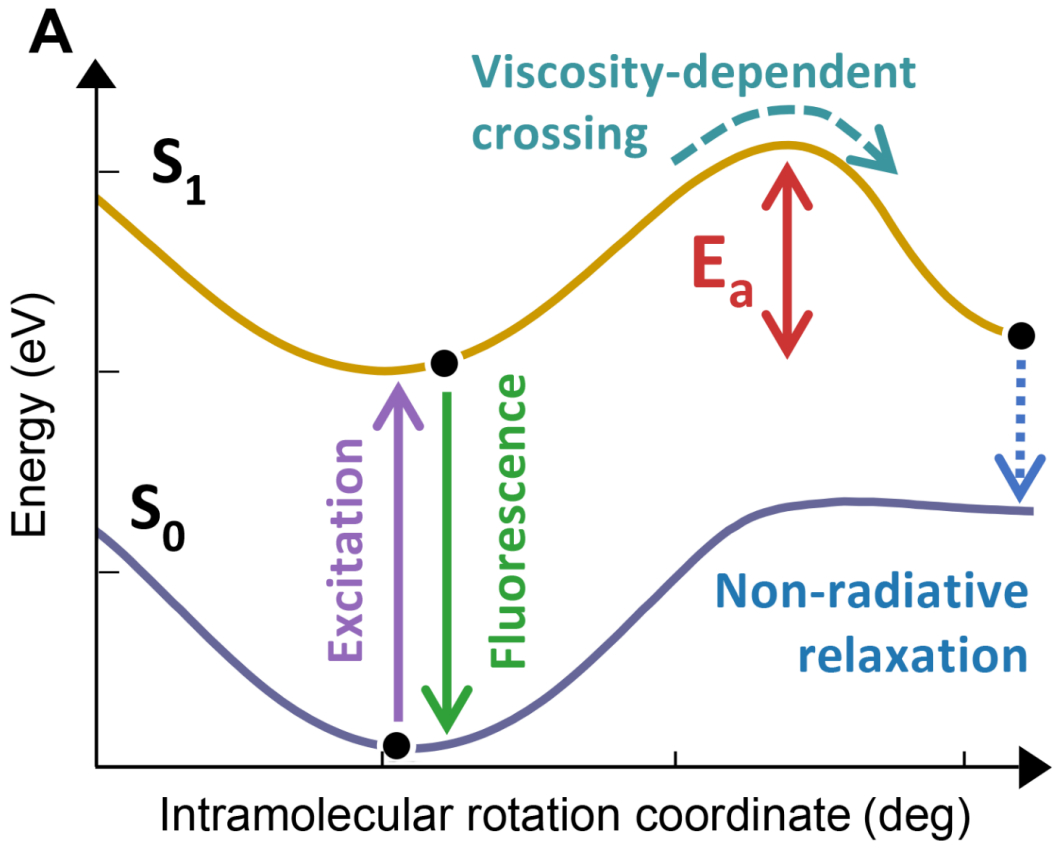
- S_0 optimization (*typical*)
  - 5 h CPU, 10 min wall
- S_1 optimization
  - 40 h CPU, 2 h wall
- S_1 PES scan
  - 480 h CPU, 24 h wall

- PCM comparison set
  - 1404 days CPU, 68 d node



Computing cost – solvent shell

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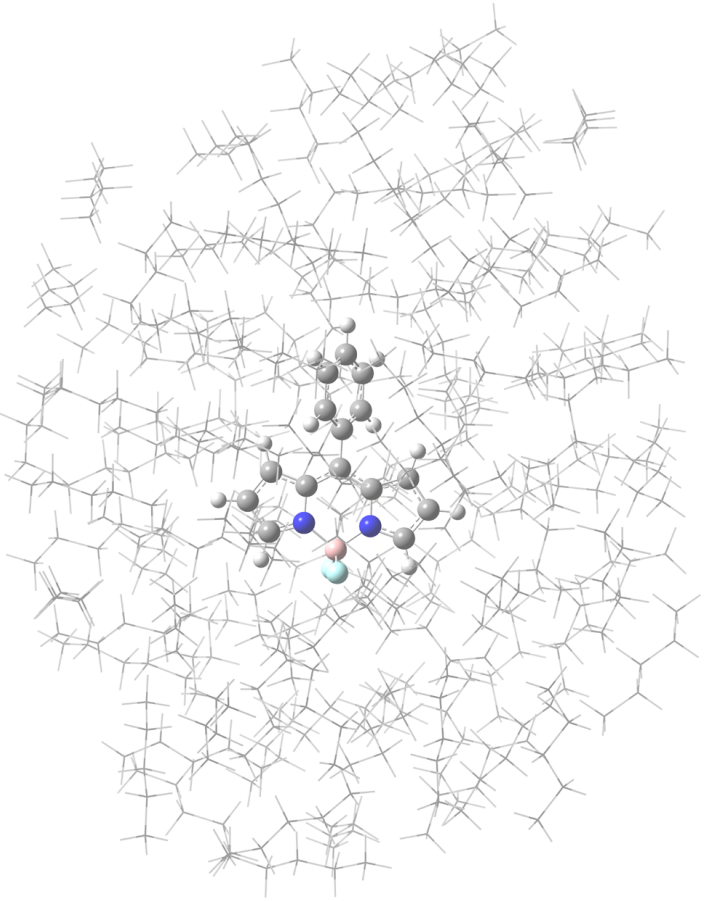
- ONIOM (DFT/MM)
  - 30-50 % additional time
- Supershell (DFT)
  - Scales as $K^{>2}$ w.r.t. basis functions
- Solvent positioning
  - MD preoptimization is needed



Computing cost – membrane MD

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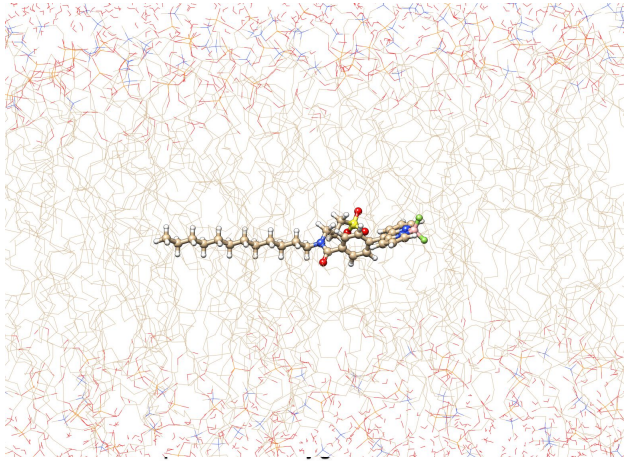
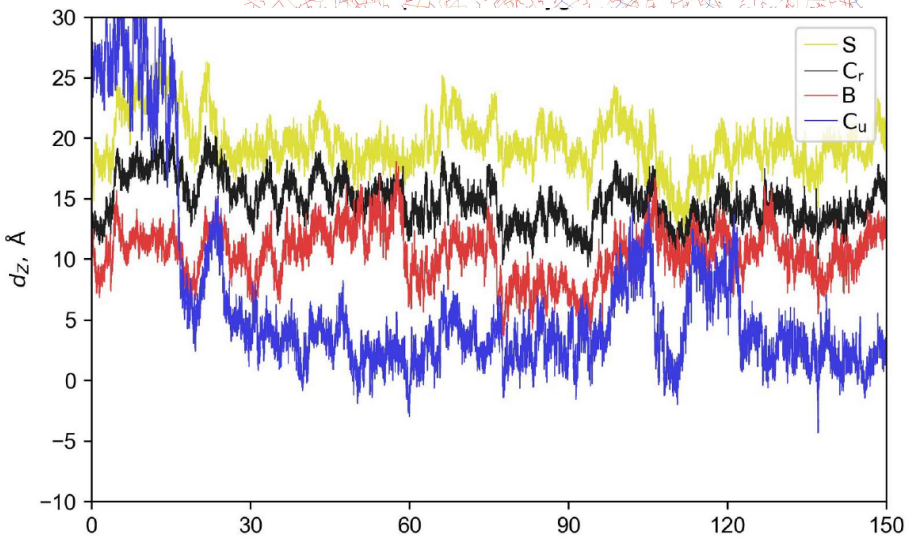
- MD run, 150 ns
  - CPU (2 nodes, 128 cores)
  - 2400 h CPU, 19 h wall
  - 191 ns / day
- MD run, 300 ns
  - Consumer GPU (RTX 3070)
  - 43 h GPU / wall
  - 167 ns / day





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Acknowledgments

- D. Narkevičius – polarity, membrane dynamics
- A. Polita – past and ongoing experimental studies
- A. Vyšniauskas, K. Maleckaitė and others – previous work

- ***Resources***: VU HPC „Saulėtekis“ (Faculty of Physics location)
- ***Support***: Research Council of Lithuania (LMT grant no. S-MIP-23-48)

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Interested? JOIN US!

- Masters, PhD, post-doc
- Research collaboration
  - esp. MD runs and analysis

Contact →

THANK YOU!

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EuroHPC Joint Undertaking
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