Dansk Fysisk Selskab

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Simulating time-resolved X-ray experimental observables from ensembles of dynamically evolving molecular structures following photo-excitation

The combination of the two monomers benzothiadiazole (BT) and thiophene (T), acting as a light-absorbing unit, is an interesting research area of polymer photovoltaics. Understanding the unit BT-1T could potentially reveal a fundamental insight in the ultrafast dynamics during a photoinduced process. By combining quantum mechanical and molecular dynamics (MD) computer simulations we can facilitate this insight of how the molecular structure theoretically evolves following an excitation of the electronic system. MD is primarily used for the investigation of the excited-state solvation structure of BT-1T through classical MD simulations in terms of the solvent-solvent and solute-solvent radial distribution functions (RDFs).

Primary authors: BIANCA, Hansen (Technical University of Denmark); Mr KRISTIAN, Nielsen (Technical University of Denmark)

Co-authors: Mr KRISTOFFER, Haldrup (Technical University of Denmark); Prof. MARTIN MEEDOM, Nielsen (Technical University of Denmark); Prof. JENS WENZEL, Andreasen (Technical University of Denmark)

Presenters: BIANCA, Hansen (Technical University of Denmark); Mr KRISTIAN, Nielsen (Technical University of Denmark)