



Showcasing research from the Computational PhotoChemistry Group led by Professor Müller at the Friedrich-Alexander-Universität Erlangen-Nürnberg, Bavaria, Germany.

shnitsel-tools: a toolkit for the full lifecycle of surface hopping trajectory data

Trajectory surface hopping (SH) simulations are widely used to study excited-state dynamics, but extracting mechanistic insight often requires extensive manual analysis and custom scripts. We introduce shnitsel-tools, a software package that enables automated, reproducible workflows for analyzing, filtering, and visualizing SH data. Applicable across diverse systems and methods, the toolkit supports systematic comparisons and benchmarking, and helps identify key parameters governing photoinduced processes.

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As featured in:



See Carolin Müller *et al.*,
Digital Discovery, 2026, **5**, 2016