

Documentation

Dataset for manuscript "High-harmonic generation from two weakly coupled molecules: a simple tight-binding model"

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1 General Information

Dataset title:	Dataset for manuscript "High-harmonic generation from two weakly coupled molecules: a simple tight-binding model"
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Type:	Simulation results
Language:	English
Rights:	CC BY-NC 4.0
DOI of the repository:	10.18453/rosdok_id00005053
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2 Description

This dataset provides the data for all figures, which are discussed in the publication [1]. Simulation parameters and details are explained therein.

3 Usage

The data is provided in the form of ".txt"-files containing the research data in tables. It can be easily accessed in python with the numpy library using the "numpy.loadtxt("filename.txt")" command or in matlab with "readtable("filename.txt")". All entries use double-precision floats. Minimal plotting examples requiring the packages pythone3, numpy, and matplotlib are provided.

4 Repository Structure

The data is grouped into the following sub-folders and files:

```
HHG_Two_Mol_TB_Repository
├── Fig1_Sketch
│   └── Eigenenergies.txt
├── Fig2_Polarization_Dependent_Yield
│   ├── Fig2_Harmonic_Order_Numbering.txt
│   ├── Fig2_Intensities_Normed.txt
│   ├── Fig2_Polarization_Phi.txt
│   └── Minimal_Plot_Data2.py
├── Fig3_HHG_Spectra_Perpendicular
│   ├── Fig3_Harmonic_Order.txt
│   ├── Fig3_Spectrum_Perp_Inter.txt
│   ├── Fig3_Spectrum_Perp_Mol.txt
│   └── Minimal_Plot_Data3.py
├── Fig4_Yield_Maximizing_Polarization
│   ├── Fig4a_Harmonic_Order_Numbering.txt
│   ├── Fig4a_Intensities_Normed.txt
│   ├── Fig4a_Polarization_Phi.txt
│   ├── Fig4b_Harmonic_Order_Numbering.txt
│   ├── Fig4b_t1s.txt
│   ├── Fig4b_Yield_Maximizing_Phi.txt
│   ├── Minimal_Plot_Data4a.py
│   └── Minimal_Plot_Data4b.py
├── Fig5_HHG_Scaling_t1s
│   ├── Fig5_Harmonic_Order_Numbering.txt
│   ├── Fig5_Intensities_Perp_Inter.txt
│   ├── Fig5_Intensities_Perp_Mol.txt
│   ├── Fig5_t1s.txt
│   └── Minimal_Plot_Data5.py
└── Fig6_HHG_Spectra_Adiabatic
    ├── Fig6_Harmonic_Order.txt
    └── Fig6_Spectrum_Adiainter.txt
```

- Fig6_Spectrum_Adiaintra.txt
 - Fig6_Spectrum_Exact.txt
 - Minimal_Plot_Data6.py
- Fig7_Polarization_Dependent_Yield_Adiabatic
 - Fig7_Harmonic_Order_Numbering.txt
 - Fig7_Intensities_Normed.txt
 - Fig7_Polarization_Phi.txt
 - Minimal_Plot_Data7.py
- Fig8_Yield_Maximizing_Polarization
 - Fig8_Harmonic_Order_Numbering.txt
 - Fig8_t1s.txt
 - Fig8_Yield_Maximizing_Phi.txt
 - Minimal_Plot_Data8.py
- Fig9_HHG_Scaling_t1s_Adiabatic
 - Fig9_Harmonic_Order_Numbering.txt
 - Fig9_Intensities_Perp_Inter.txt
 - Fig9_Intensities_Perp_Mol.txt
 - Fig9_t1s.txt
 - Minimal_Plot_Data9.py

References

- [1] Lina Bielke, Samuel Schöpa, Falk-Erik Wiechmann, Franziska Fennel, Dieter Bauer, *High-harmonic generation from two weakly coupled molecules: a simple tight-binding model*, Phys. Rev. A, 10.1103/7ljs-sbpy (2026)