

ONETEP Tutorials 7.0.0

Introduction

Welcome to ONETEP's Tutorials!

This is a privately maintained repository of tutorials of ONETEP. The aim of this repository is to make the tutorial easier to read by including additional tutorials and using mkdocs.

Contents:

- Tutorial 1: Setting up Simple ONETEP Calculations
- Tutorial 4: Geometry optimization
- Tutorial 5: DFT+U on strongly correlated magnetic materials: A case study on antiferromagnetic Hematite
- Tutorial 6: Time-Dependent DFT
- Tutorial 8: Implicit solvation, visualisation and properties: Protein-ligand free energy of binding for the T4 lysozyme
- Tutorial 9: Analysis and visualization
- Tutorial 10: Simulation cell relaxation
- Tutorial 11: Electrified electrode-electrolyte interfaces under potentiostatic control
- Tutorial 12: Quantum embedding with (time-dependent) embedded mean-field theory: hydrogenation and excitations of pentacene
- Tutorial 13: ASE ONETEP interface
- Tutorial 14: Electron Energy Loss Spectroscopy in ONETEP

