

# PHYS-E0546 Density-Functional Theory D

## Project Proposal

*No more than 2 pages*

**Project title:**

**Your name:**

**Department:**

### 1. Project description

Context and background

*Briefly describe the problem you would like to solve and its context. (Delete this text, when you fill out the box.)*

DFT contribution

*Describe how the problem can be broken down into steps that can be tackled with DFT. (Delete this text, when you fill out the box.)*

Expected outcome

*Briefly describe the results you expect and how they could contribute to the solution of your problem (and to your field in general). (Delete this text, when you fill out the box.)*

## 2. Computational methodology

### Calculations

*Please name the DFT code you are planning to use and describe the types of DFT calculations for your project (e.g. total energies (e.g. for conformer search), total energy differences (e.g. for cohesive energies), geometry optimization, molecular dynamics, etc.). Also think which scripts (if any) you might need, whether you have to modify them or even write new scripts. (Delete this text, when you fill out the box.)*

### Computational budget

*Please estimate roughly how feasible your project is based on the computational scaling laws that were shown in the lecture. You can estimate base times for small systems or take them from the tutorial exercises. (Delete this text, when you fill out the box.)*

## 3. Work plan

Please sketch out the tasks for each week of the project (e.g. prepare atomic geometries, run calculation for structure xyz, analyze data, write report).

	Task
Week 1	
Week 2	
Week 3	
Week 4	
Week 5	
Week 6	