FHI-aims Tutorial Series 2021

Properties of Materials from First Principles
A Virtual Hands-on Tutorial Using FHI-aims

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Hands-on Tutorial 1

Basics of Running FHI-aims

Hands-on Tutorial

Prerequisites

- A computer/laptop with at least **2 cores and 4GB RAM** (however, the more the better) with Linux/Mac OS
- An installed **FHI-aims executable** with the version **210716_1**.

  Get the code here: fhi-aims.org
- working **python3** (version 3.7>=) installation on your machine to use all of the tutorial tools

Hands-on Tutorial

Material

- Tutorial Instructions:

  https://fhi-aims-club.gitlab.io/tutorials/basics-of-running-fhi-aims

- Tutorial Solutions:

  https://gitlab.com/FHI-aims-club/tutorials/basics-of-running-fhi-aims

- Tutorial Communication: Slack Workspace

  fhiaimstutori-ypu5815.slack.com

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Tools

- GIMS: Graphical Interface for Materials Simulations

  https://gims.ms1p.org

- CLIMS: Command-Line Interface for Materials Simulations

  `pip install clims` (on a cluster: `pip install --user clims`)

Hands-on Tutorial

Objectives

How to run DFT calculations for molecules and solids

- The FHI-aims input files `geometry.in` and `control.in`
- The FHI-aims species defaults
- Running FHI-aims in parallel
- Structure of the main output file
- Difference for systems with and without (collinear) spin
- Structure relaxation for non-periodic and periodic systems

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Content

1. **Non-spinpolarized, non-periodic systems (H2O):**
   Understanding in- and output files, performing structure optimization

2. **Spinpolarized, non-periodic systems (O2):**
   Spin initialization

3. **Periodic systems (Si and GaAs structure):**
   Relaxation, Post-processing (densities of states, band structure, Mulliken-projected band structure)

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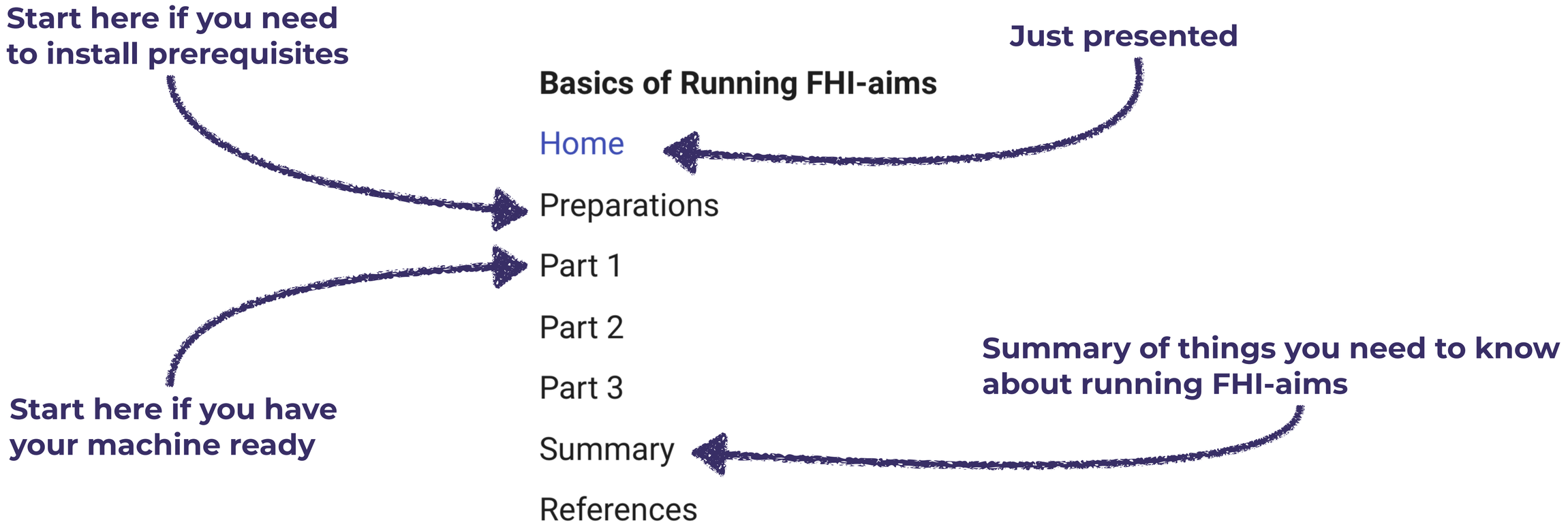
Course

- https://fhi-aims-club.gitlab.io/tutorials/basics-of-running-fhi-aims



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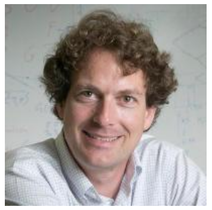
Tutors and How to Reach us



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Raise your voice on zoom or
use the Slack workspace for questions