Leopold Talirz

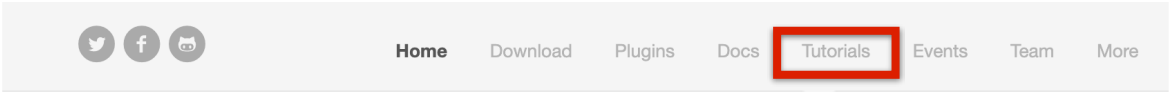
# AiiDA tutorial

| | |
|---|---|
| 9:30-10:30 | Introductory lecture |
| 10:50-12:20 | Getting set up &<br>a "first taste" of AiiDA |
| 12:20-14:00 | Lunch |
| 14:00-15:50 | Extended AiiDA tutorial<br>Go at your own speed |
| 16:10-17:10 | Advanced tutorial continued<br>Available for Q&A |

# Tutorial Team

- Leopold Talirz (EPFL)
- Juson Yu (South China University of Technology)
- Yunpei Liu (Xiamen University)
- Jingfang Xiong (Xiamen University)

# Let's head to aiida.net




AiiDA

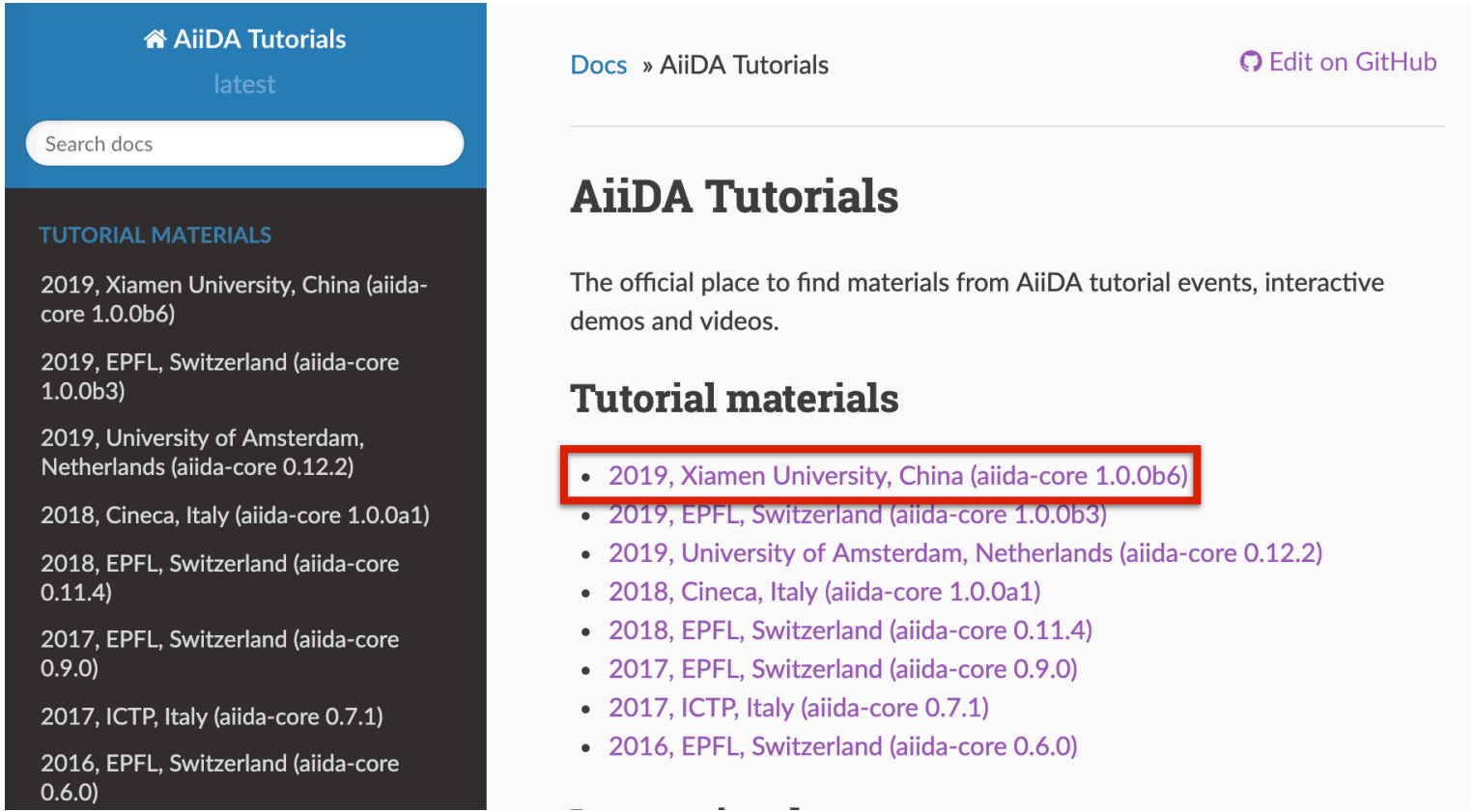
**Automated Interactive Infrastructure and Database for Computational Science**

AiiDA is a flexible and scalable informatics' infrastructure to manage, preserve, and disseminate the simulations, data, and workflows of modern-day computational science. Able to store the full provenance of each object, and based on a tailored database built for efficient data mining of heterogeneous results, AiiDA gives the user the ability to interact seamlessly with any number of remote HPC resources and codes, thanks to its flexible plugin interface and workflow engine for the automation of complex sequences of simulations.

**Journal ref**: G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, and B. Kozinsky, AiiDA: automated interactive infrastructure and database for computational science, Comp. Mat. Sci. 111, 218-230 (2016)

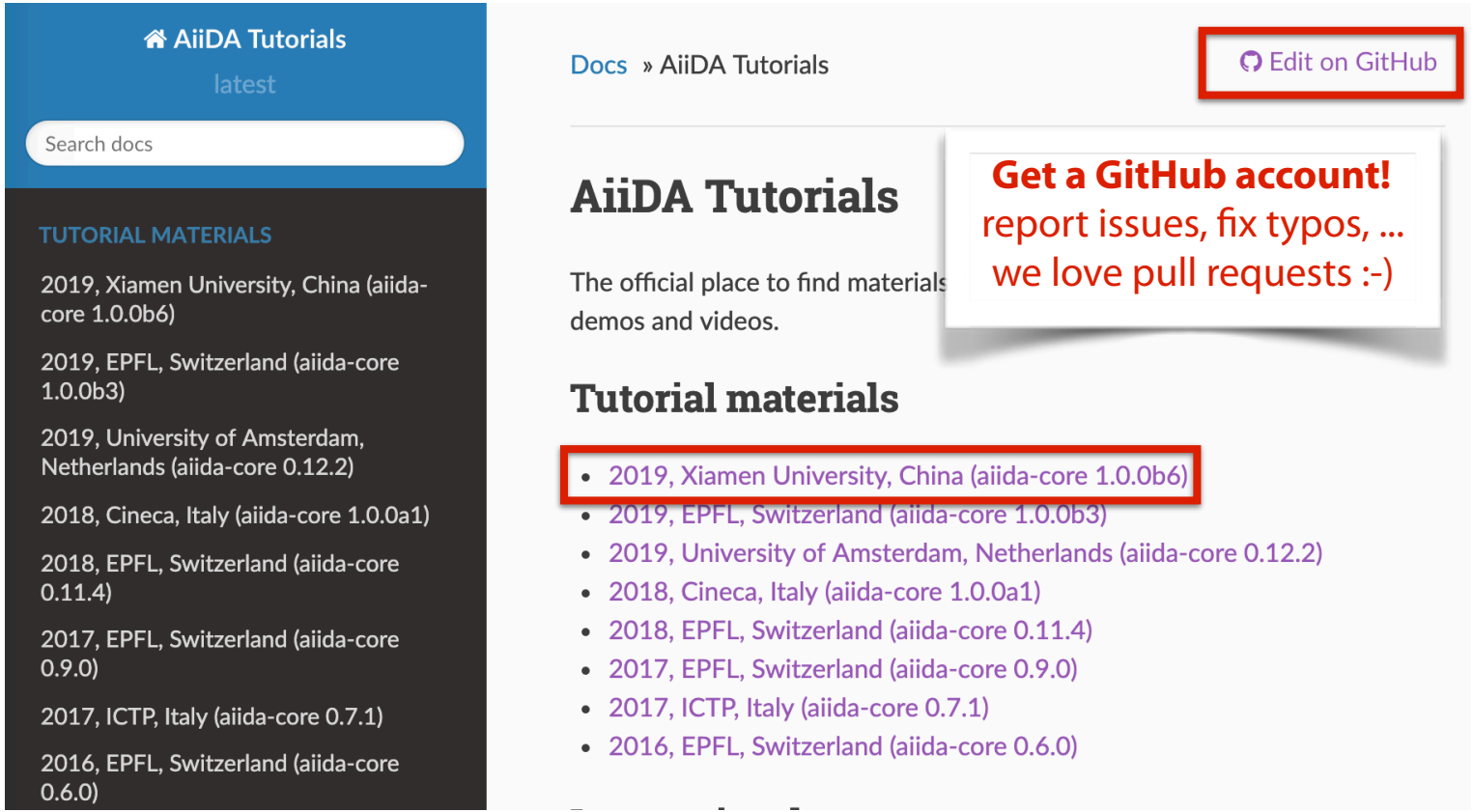
**Open access link:** arXiv:1504.0116

# Tutorial materials




**aiida-tutorials.readthedocs.io**

# Tutorial materials

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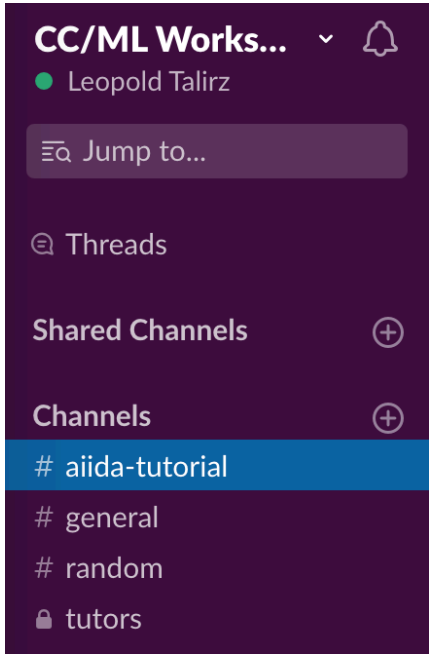
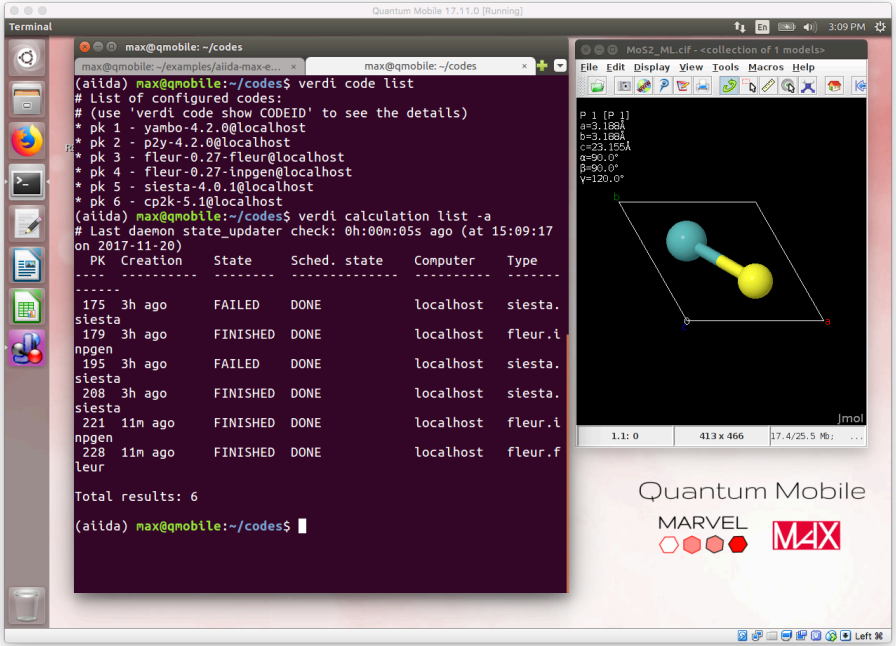
# Important information




- If possible, **create a WiFi hotspot using your phone** - it seems Huawei cloud blocks when too many use the local WiFi
- Feel free to ask questions on slack
  **invite link:** dwz.cn/WPIahDr5
  **(capital i, not lowercase L)**
- **Password for "max" user of your tutorial virtual machine**
  **XMNAiiDA2019**

# Questions?

# Quantum Mobile Virtual Machine




- Ubuntu 18.04 LTS
- **AiiDA & AiiDA Lab**
- **Open-source codes: Quantum ESPRESSO, Siesta, fleur, yambo, cp2k, Wannier90 + AiiDA plugins**
- Great for tutorials & lectures (EPFL, ETHZ, ICTP, MolSim and online classes: compmatphys.org)
- **Modular setup using ansible**

Runs on any Linux, MacOS and Windows hosts using VirtualBox

**Download**: materialscloud.org/work/quantum-mobile