Materials Science Colloquium (Hybrid)

TECHNISCHE UNIVERSITÄT DARMSTADT

Monday, February 12, 2024, 15:20, Room 77 & Zoom

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FAIR Research Data Management for Materials Scientists using NOMAD

Abstract

The Novel Materials Discovery Laboratory (NOMAD) [nomad-lab.eu] is an online, open data infrastructure tailored towards searching and publishing materials science data. NOMAD already supports an array of computational codes and techniques, with over 50 parsers that automatically extract essential (meta)data from the raw output of standard calculations. Traditionally, the NOMAD repository has focused on contributions from Density Functional Theory (DFT) calculations, accumulating over 13 million such entries. More recently, this framework has been expanded considerably, now supporting advanced many-body calculations and molecular dynamics simulations, as well as experimental synthesis and characterization techniques.

During this talk, I will first introduce basic concepts in Research Data Management and the F.A.I.R. principles [1]. Then, I will talk about the specific project which I belong to, FAIRmat, and what our objectives are. I will show the latest NOMAD capabilities and how you can use this software for data management in your group or department. Then, I will give a practical hands-on session on the basics of using NOMAD.

[1] Visit: https://www.go-fair.org/fair-principles/

Organization WiSe 23/24: Alff/Hofmann Get-together after the lecture with drinks and pretzels

https://tu-darmstadt.zoom.us/j/64148750805?pwd=eUcyd2M5a1FaWVdiN3ZOR2I2Mm5XUT09

Meeting-ID: 641 4875 0805, Code: 716255