

Ontologies for Materials-Databases Interoperability (OMDI2021)

Tuesday, Oct 5 (all times in CEST)

8:50 - 9:00 - *Logging in*

9:00 - 9:05 - *Opening and welcome*

Ontologies and their place in open science (chair: Rickard Armiento)

9:05 - 9:45 - Peter Murray-Rust

Scientific Ontologies in the Digital Age

9:55 - 10:35 - Emanuele Ghedini

Philosophy, Methods and Ambitions of the EMMO: the Elementary Multiperspective Material Ontology.

10:45 - 11:00 - *Coffee*

11:00 - 11:40 - Session discussion

11:40 - 11:50 - *Short break*

11:50 - 12:30 - Session discussion continued

Lunch - *Online meeting active for digital lunch together*

Ontologies for data exchange (chair: Matthias Scheffler)

14:00 - 14:20 - Elsa Olivetti

The Need for Ontologies in Materials Text and Data Mining

14:25 - 14:45 - Luca Ghiringhelli

Ontologies in Computational Materials Science: The NOMAD experience

14:50 - 15:10 - Patrick Lambrix

Lessons learned for developing ontologies

15:15 - 16:00 - Session discussion

16:00 - 16:20 - *Coffee*

Ontologies for data exchange II (chair: Anthony Scemama)

16:20 - 16:40 - Gian-Marco Rignanese

The OPTIMADE REST API for Querying Materials Databases: Challenges and Opportunities

16:45 - 17:05 - Cormac Toher

Ontologies for materials properties and structures in AFLOW

17:10 - 17:20 - *Short break*

17:20 - 17:40 - Ellad Tadmor

Standard Access to Datasets for Training Interatomic Potentials

17:40 - 18:30 - Session discussion

18:30 - 19:30 - Poster session

Wednesday, Oct 6

8:55 - 9:00 - Welcome

Ontologies in materials science (chair: David Cebon)

9:00 - 9:20 - James Hester

The Crystallographic Information Framework: a relational data ontology for scientific programmers

9:25 - 9:45 - Toshihiro Ashino

Materials Ontology: An Infrastructure for Exchanging Materials Information and Knowledge

9:50 - 10:40 - Session discussion

10:40 - 11:00 - Coffee

Ontologies in materials science II (chair: Gareth Conduit)

11:00 - 11:20 - Saulius Gražulis

Needs for ontologies for experimental databases – experience of the COD

11:25 - 11:45 - Casper W. Andersen

Ontologies for Crystallography

11:50 - 12:40 - Session discussion

Lunch - Online meeting active for digital lunch together

Ontologies for materials properties (chair: Nicola Marzari)

14:00 - 14:20 - Steve Collins

Ontologies for Photon and Neutron Science

14:25 - 14:45 - Giovanni Pizzi

Ontology-driven simulations with AiiDA and common workflows

14:50 - 15:10 - Huanyu Li

An Ontology for the Materials Design Domain

15:15 - 16:05 - Session discussion

16:05 - 16:20 - Coffee

Ontologies for materials properties II (chair: Stefano Curtarolo)

16:20 - 16:40 - Zachary Trautt

Exploring FAIR Digital Objects within Materials Science and Engineering

16:45 - 17:05 - Donny Winston

The Materials Research Data Alliance (MaRDA) Data Dictionaries Working Group: A Progress Report

17:10 - 17:20 - Short break

17:20 - 17:40 - Matthew Horton

Propnet: A Knowledge Graph for Materials Science

17:45 - 18:30 - Session discussion

Dinner - Dinner for in-person participants

Thursday, Oct 7

8:55 - 9:00 - *Welcome*

Ontologies for data integration (chair: Gian-Marco Rignanes)

9:00 - 9:20 - **Davide Di Stefano**

Materials Databases and Ontology: a perspective

9:25 - 9:45 - **Yoav Nahshon**

SimPhoNy: An ontology-driven Python framework for promoting interoperability of materials science applications

9:50 - 10:40 - **Session discussion**

10:40 - 11:00 - *Coffee*

Ontologies for data integration II (chair: Luca Ghiringhelli)

11:00 - 11:20 - **Evgeny Blokhin**

Tackling the OWL2 complexity using the Python interface to the FaCT++ reasoner

11:25 - 11:45 - **Thomas Hagelien**

SOFT/DLite - Applications of ontologies

11:50 - 12:40 - **Session discussion**

Lunch - *Online meeting active for digital lunch together*

Ontology use in applications (chair: Gerhard Goldbeck, Daniele Toti)

14:30 - 14:50 - **Gareth Conduit**

Ontologies for machine learning driven materials design

14:55 - 15:35 - **Session discussion**

15:35 - 16:00 - *Coffee*

16:00 - 16:20 - **Chris Mungall**

Experiences in the biosciences with the Open Biological Ontologies Foundry and the Gene Ontology

16:25 - 18:00 - **Synopsis, outlook, and goodbye**