

## 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**

Page 1/3

# Program

OMDI2021

**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

Page 2/3



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# Program

OMDI2021

**Thursday, Oct 7**

**8:55 - 9:00 - Welcome**

**Ontologies for data integration** (*chair: Sara Bonella*)

**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**