FAIR-DI European Conference on Data Intelligence 2024

Monday, October 28, 2024

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (8:45 AM - 10:30 AM)

time	[id] title	presenter
8:45 AM	[67] Active learning for data-efficient optimisation of materials and processes	TODOROVIC, Milica
9:25 AM	[107] The research data life cycle in experimental solid-state physics: challenges, strategies and solutions	WEBER, Heiko
9:45 AM	[93] The MSE-KG: Navigating the MatWerk consortium for Materials Science Discoveries	NOROUZI, Ebrahim
10:05 AM	[99] OFED@NFFA-DI	BAZZOCCHI, Federica

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (11:00 AM - 1:00 PM)

time	[id] title	presenter
11:00 AM	[60] Auto-generated Materials Databases and Language Models	COLE, Jacqui
11:40 AM	[110] Towards interoperable materials-science (meta)data: the NOMAD taxonomy of materials properties	GHIRINGHELLI, Luca
12:00 PM	[69] FAIR Data Management for Computational Materials Science using NOMAD	Dr RUDZINSKI, Joseph F.
12:20 PM	[17] Building Knowledge Graphs with the ELN Herbie	KIRCHNER, Fabian
12:40 PM	[16] Customisable open-source research data management system for high-throughput experimentation and collaborative projects in materials science	Dr DUDAREV, Victor

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (2:00 PM - 4:00 PM)

time	[id] title	presenter
2:00 PM	[61] From Specialist to Generalist Models in AI: The Role of Data and Physics	SANDFELD, Stefan
2:40 PM	[95] Integrating analysis and ML applications within digitalized workflows for experimental materials science	KAPOOR, Sarthak
3:00 PM	[13] RDM-desktop - a helper for data management on a PC	HARASZTI, Tamás
3:20 PM	[73] Kadi4Mat: Automated Extraction of Structure-Property Linkages using AI	GRIEM, Lars
3:40 PM	[96] ALPmat: A platform for accelerating materials design via optimized knowledge exploitation and sample efficiency	Dr SPITALER, Jürgen

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (4:30 PM - 6:30 PM)

time	[id] title	presenter

4:30 PM	[62] Transforming chemistry with transformers	JABLONKA, Kevin
5:10 PM	[97] RefXAS database: Metadata Fields, Quality Criteria and Data formats	Dr GAUR, Abhijeet
5:30 PM	[100] RefXAS database: Technical developments and features	PARIPSA, Sebastian
5:50 PM	[18] tomato: incremental au-tomation for your lab, without the pain!	KRAUS, Peter
6:10 PM	[105] Representation of computational materials and simulation workflows – leveraging ontologies and knowledge graphs	Dr AZOCAR GUZMAN, Abril

Tuesday, October 29, 2024

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (8:45 AM - 10:30 AM)

time	[id] title	presenter
8:45 AM	[63] Machine-learning you can trust: interpretability and uncertainty quantification in chemical machine learning	CERIOTTI, Michele
9:25 AM	[84] Dynamic multi-fidelity decision-making for self-driving labs	FRIEDERICH, Pascal
9:45 AM	[19] Digital twin for a nanophotonic chiral sensing platform	NYMAN, Markus
10:05 AM	[123] FAIR-DI Award for data handling in a PhD thesis	

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (11:00 AM - 1:00 PM)

time	[id] title	presenter
11:00 AM	[64] AI-ready materials science data	MARQUEZ, Jose
11:40 AM	[94] NFDI4DS Ontology: The NFDI for Data Science Ontology	Dr GESESE, Genet Asefa
12:00 PM	[88] IN DEEP: INterdisciplinary DatabasE for Explainable Peptide prediction	Dr GOMEZ FLORES, Claudia Leticia
12:20 PM	[20] A data format for T-matrices in optics and photonics	ASADOVA, Nigar
12:40 PM	[98] An Ontology for Vapor Deposition Implemented as a Data Schema in NOMAD	NÄSSTRÖM, Hampus

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time	[id] title	presenter
2:00 PM	[65] Correlative characterization and data science in functional materials	TOMA, Francesca
2:40 PM	[104] Automated local solutions for FAIR data in catalysis	MOSHANTAF, Abdulrhman
3:00 PM	[86] Advancing Catalysis Research through Digitalization: The Role of NOMAD in Facilitating Data Management and Analysis	SCHUMANN, Julia
3:20 PM	[92] Database-Driven Discovery of Molecular Catalysts for Efficient Water Electrolysis	CLARKE, Cian
3:40 PM	[91] New Computational Approaches for Navigating the Deep Chemical Space of Transition Metal Complexes	SOMMER, Timo

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (4:30 PM - 6:30 PM)

time	[id] title	presenter
4:30 PM	[66] The Role of Data Intelligence in Chemistry Research Data Infrastructures	JUNG, Nicole
5:10 PM	[106] Coupling software tools for reproducible data analysis workflows in Atom Probe Tomography	Dr MENON, Sarath
5:30 PM	[71] Data-driven inverse design of magnetic materials	CHAUDHARY, Vikrant
5:50 PM	[75] Reviving the Perovskite Solar Cell Database: Creating a Living Database with Large Language Models	SHABIH, Sherjeel

6:10 PM	[78] FAIR Data Workflow for High-Throughput Combinatorial Exploration of Novel Halide Perovskites	UNOLD, Thomas

Wednesday, October 30, 2024

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (8:45 AM - 10:30 AM)

time	[id] title	presenter
9:25 AM	[108] Accelerating MOF Synthesis via AI Integration	Dr TSOTSALAS, Manuel
9:45 AM	[11] MOFGalaxyNet: Bridging AI Modeling and Social Networking for Predicting Guest Accessibility in Metal-Organic Frameworks	JALALI, Mehrdad
10:05 AM	[111] Determination of the rate-limiting steps of hydride absorption/desorption reactions aided by unsupervised machine learning algorithm	NEVES, A.

Session - click on "Detailed view" on the top right to see all contributions - Kurfürstensaal (11:00 AM - 1:00 PM)

time	[id] title	presenter
11:00 AM	[68] Accelerating formulation design by understanding the physical properties of complex molecular ensembles	ROBINSON, William
11:40 AM	[115] The status of NeXusFormat implementation in ALBA Synchrotron	SAIZ, Fernan
12:00 PM	[117] Deep learning of optical spectra of semiconductors and insulators	GROSSMANN, Max
12:20 PM	[118] Leveraging RAG Architecture and Kadi4Mat Integration to Develop an Advanced Research Assistant Chatbot for Scientific Publications	ZHAO, Yinghan
12:40 PM	[119] Operating complex data analysis workflows in materials science online via a chatbot	KOCH, Christoph