

PROGRAM OF WORKSHOP DACOMSIN: DATA AND COMPUTATION FOR MATERIALS SCIENCE AND INNOVATION

October 26, 2021

Place: NUST MISIS, online MS Teams

Time	Event
9:00-10:30 (Moscow time)	Registration time. Check connections.
10:30-10:45	Ceremony of Opening of the Workshop
	Session “Machine Learning for Materials Science”
10:45-11:05	Yi Liu (Shanghai University) Machine Learning Accelerated Multicomponent Alloy Design
11:05-11:25	Nadezhda N. Kiselyova (IMET RAS); Victor A. Dudarev (NRU HSE); Andrey V. Stolyarenko (IMET RAS) Machine Learning Application to Predict New Inorganic Compounds – Results and Perspectives
11:25-11:45	Matteo Baldoni; Fabio Le Piane; Francesco Mercuri (CNR-ISMN) Artificial intelligence, machine learning and data-enabled multiscale simulation workflows for the design and development of molecular materials
11:45-12:05	Jakob Ropers, Marco M. Mosca, Olga Anosova, Vitaliy Kurlin, and Andrew I. Cooper (University of Liverpool) Fast predictions of lattice energies by continuous isometry invariants of crystal structures
12:05-12:25	Faridun Jalolov; Artem Oganov; Alexander G Kvashnin (Skolkovo Institute of Science and Technology) Simulations of mechanical properties of materials by using machine learning interatomic potentials
12:25-12:40	Break
12:40-13:25	Johan Bratberg, Vice President, Thermo-Calc Software AB The role of CALPHAD-bases tools in filling the materials data gaps for materials 4.0.
	Session “Databases on Properties of Substances and Materials”
13:25-13:45	Toshihiro Ashino (Toyo University); Nobutaka Nishikawa (Mizuho Research & Technologies, Ltd.); Masahiko Demura (National Institute for Materials Science (NIMS)); Takuya Kadohira (NIMS) Implementation of Materials Data Integration using Ontology
13:45-14:05	Fabio Le Piane (ISMN-CNR); Matteo Baldoni (ISMN-CNR); Mauro Gaspari (University of Bologna); Francesco Mercuri (ISMN-CNR) Molecular and Materials Basic Ontology: development and first steps
14:05-14:25	Martin T. Horsch (High Performance Computing Center Stuttgart (HPCCS)); Taras Petrenko (HPCCS); Volodymyr Kushnarenko (HPCCS); Björn Schembera (HPCCS); Bianca Wentzel (Fraunhofer Institute for Open Communication Systems (FIOCS)); Alexander Behr (TU Dortmund); Norbert Kockmann (TU Dortmund); Sonja Schimmler (FIOCS); Thomas Bönisch (HPCCS) Interoperability and architecture requirements analysis and metadata standardization for a research data infrastructure in catalysis
14:25-15:10	Lunch
15:10-15:30	Victor A. Dudarev; Sergey Babikov (NRU HSE) Searching for an Optimal Data Platform for Relevant Information Search in Inorganic Chemistry and Materials Science
15:30-15:50	Reetu Elza Joseph (Karlsruhe Institute of Technology (KIT)); Aditya Chauhan (KIT); Catriona Eschke (Helmholtz-Zentrum Hereon); Ahmad Zainul Ihsan (Forschungszentrum Jülich); Mehrdad Jalal (KIT); Ute Jäntsche (KIT); Nicole

	Jung (KIT); C. N. Shyam Kumar (CEA Saclay); Christian Kübel (KIT); Christian Lucas (Helmholtz-Zentrum Hereon); Matthias Mail (KIT); Andrey Mazilkin (KIT); Charlotte Neidiger (KIT); Mirco Panighel (Consiglio Nazionale delle Ricerche - Istituto Officina dei Materiali); Stefan Sandfeld (Forschungszentrum Jülich); Rainer Stotzka (KIT); Richard Thelen (KIT); Rossella Aversa (KIT) Metadata Schema to support FAIR Data in Scanning Electron Microscopy
15:50-16:00	Break
	Session “Computational Materials Science”
16:00-16:20	Alexander G. Kvashnin (Skolkovo Institute of Science and Technology (SIST)); Dmitry Rybkovskiy (SIST); Vladimir Filonenko (High Pressure Physics Institute (HPPI)); Vadim Brazhkin (HPPI); Artem Oganov (SIST) Computational prediction, Synthesis, Properties, and Crystal Structure of WB5-x
16:20-16:40	Alexey L. Voskov (Lomonosov Moscow State University) Usage of Robust Regression for Approximation of Thermodynamic Data
16:40-17:00	Tao Fan (Skolkovo Institute of Science and Technology) AICON2: A program for calculating transport properties quickly and accurately
17:00-17:20	Closing Ceremony