Modern trends in Computational Materials Discovery

17 - 21 November 2022
Isfahan University of Technology, Isfahan, Iran

It is a joint workshop between the USPEX group and the Physics department of the Isfahan University of Technology (IUT) aiming to train modern computational methods for discovering new materials and predicting material properties. The workshop program contains scientific lectures in the morning sessions and hands-on tutorials in the afternoons. The hands-on sessions are mainly devoted to USPEX, as a pioneering package for material design in the framework of evolutionary algorithms.

Main Topics

- DFT and electronic structure
- Machine learning and Data science
- Novel material properties
- Magnetic materials
- Evolutionary algorithm and global optimization
- Materials discovery and design

Organizers

Artem R. Oganov (Skoltech)
Mojtaba Alaei (IUT)

Local Organizers

Ismaeil Abdolhosseini Sarsari
Mojtaba Alaei (chair)
S. Javad Hashemifar

Invited Speakers

Mojtaba Alaei, IUT, Iran
Zahed Allahyari, Skoltech, Russia
Gustav Bihlmayer, Fritz-Haber Institute, Germany
Stefano de Gironcoli, SISSA, Italy
Sergey Levchenko, Skoltech, Russia
Mehdi Neek-Amal, SRTTU, Iran
Artem R. Oganov, Skoltech, Russia
Matthias Scheffler, Fritz-Haber Institute, Germany
Sandro Scandolo, ICTP, Italy
Alexandre Tkatchenko, Uni. of Luxembourg, Luxembourg

Deadline online registration:
September 30, 2022

Website:
https://qsm.iut.ac.ir/workshop-iut-uspex

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Skoltech
Skolkovo Institute of Science and Technology

Isfahan University of Technology

USPEX Computational Materials Discovery

The Abdus Salam International Centre for Theoretical Physics