



**Hands-on Workshop and Humboldt-Kolleg:
Density-Functional Theory and Beyond: Basic Principles and Modern Insights**
2-13 May 2016
Isfahan University of Technology, Isfahan, Iran



This workshop will deal with the basics and recent advances of electronic-structure theory, especially density-functional theory. The workshop morning lectures introduce basic topics, from the choice of functional basis set to ways to account for relativity, magnetism, long-range dispersion and furthermore includes advanced topics like excited-state properties, free energies, and nuclear quantum effects. In the afternoons, participants will gain experience in hands-on sessions guided by skilled tutors. The main computational workhorse for the afternoon sessions will be the FHI-aims all-electron code, which embodies all necessary methods.

Invited Speakers:

Carsten Baldauf, Fritz-Haber-Institute, Germany
Christian Carbogno, Fritz-Haber-Institute, Germany
Claudia Draxl, Humboldt Universität, Germany
Ralph Gebauer, ICTP, Italy
Luca Ghiringhelli, Fritz-Haber-Institute, Germany
Ali Hassanali, ICTP, Italy
Graeme Henkelmann, The University of Texas at Austin, USA
Oliver Hofmann, TU Graz, Austria
S. Akbar Jafari, Sharif University of Technology, Iran
Peter Kratzer, Universität Duisburg Essen, Germany
Abdollah Langari, Sharif University of Technology, Iran
Sergey Levchenko, Fritz-Haber-Institute, Germany
Fawzi Mohamed, Fritz-Haber-Institute, Germany
Mohammad R. Mohammadzadeh, University of Tehran, Iran
Eva Pavarini, Forschungszentrum Jülich GmbH, Germany
Patrick Rinke, Aalto University Helsinki, Finland
Mariana Rossi, Oxford University, UK
Angel Rubio, University of the Basque Country, Spain
Matthias Scheffler, Fritz-Haber-Institute, Germany
Markus Schneider, Fritz-Haber-Institute, Germany
Alexandre Tkatchenko, Fritz-Haber-Institute, Germany
Nahid Talebi Sarvari, Max Planck Institute, Stuttgart, Germany
Weitao Yang, Duke University, USA
Igor Ying Zhang, Fritz-Haber-Institute, Germany

Organizers:

Hadi Akbarzadeh (IUT)
Carsten Baldauf (FHI)
S. Javad Hashemifar (IUT)
Matthias Scheffler (FHI)

Local Organizers at IUT:

Ismaeil Abdolhosseini Sarsari
Hossein Ahmadvand
Mojtaba Alaei
S. Javad Hashemifar



Alexander von Humboldt
Stiftung / Foundation

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