WE-Heraeus Workshop on ab-initio methodologies
for complex magnetism and magneto-superconductivity
15-18 September 2025

Monday, 15 September

10:00-11:30
Arrival and registration

CHAIR: LÁSZLÓ SZUNYOGH
11:30-12:20
Contribution: Forces and total energies in the KKR method
Presenter: Rudolf Zeller

12:20-13:10
Contribution: Scalable First Principles Multiple Scattering Calculations for Complex Material
Presenter: Markus Eisenbach

13:10-14:30
Lunch break

CHAIR: HUBERT EBERT
14:30-14:40
Contribution: About the Wilhelm and Else Heraeus Foundation
Presenter: Stefan Jorda

14:40-15:30
Contribution: Superconductivity in altermagnets Presenter: : Annica Black-Schaffer

15:30-16:20
Contribution: Superconducting orbitronics: phase engineering, magneto-electric and nonreciprocal effects
Presenter: Mario Cuoco

16:20-16:40
Coffee break

CHAIR: JAN MINÁR
16:40-17:30
Contribution: From electronic structure to magnetisation dynamics
Presenter: Olle Eriksson

17:30-18:20
Contribution: Magnon spectroscopy of complex magnetic materials from first principles
Presenter: Manuel dos Santos Dias

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Tuesday, 16 September

CHAIR: JULIE STAUNTON

9:00-09:50

Contribution: Calculating response quantities using the KKR Green function formalism
Presenter: Hubert Ebert

09:50-10:40

Contribution: Quantum Materials and Magnetic Phenomena Studied by Spin-Resolved ARPES: Theoretical perspectives
Presenter: Ján Minár

10:40-11:00
Coffee break

CHAIR: STEFAN BLÜGEL

11:00-11:50
Contribution: Statistical physics of multi-component alloys using the KKR-CPA
Presenter: Julie Staunton

11:50-12:40
Contribution: Revealing the electronic structure of high-entropy alloys
Presenter: Stephen Dugdale

12:40-14:10
Lunch break

14:10-14:40
Contribution: Flash poster presentations

14:40-16:00

Contribution: Poster session

16:00-16:20

Coffee break

16:20-17:40

Contribution: Poster session

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Wednesday, 17 September

CHAIR: ZEILA ZANOLLI

09:00-09:50

Contribution: Electronic structure of superconducting nickelates from first-principles
Presenter: Antia Botana

09:50-10:40
Contribution: Ab initio methods for superconductivity beyond GW
Presenter: Antonio Sanna

10:40-11:00
Coffee break

CHAIR: MARIO CUOCO

11:00-11:50

Contribution: Density functional Bogoliubov-de Gennes theory for superconductors implemented in the SIESTA code
Presenter: Zeila Zanolli

11:50-12:40

Contribution: First Principles Approches to Superconducting Orbitronics and their application to chirality
Presenter: Tom G Saunderson

12:40-14:10
Lunch break

MARKUS EISENBACH

14:10-15:00
Contribution: Complex magnetism of orthorhombic iridates
Presenter: Marjana Ležaić

15:00-15:50
Contribution: Magnetocrystalline anisotropy in MnGa alloys
Presenter: Tamio Oguchi

15:50-16:10
Coffee break

STEPHEN DUGDALE

16:10-17:00
Contribution: Real-space descriptions of magnetic interactions and complex magnetism
Presenter: Anders Bergman

18:00-21:00
Conference dinner

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Thursday, 18 September

CHAIR: RUDOLF ZELLER

09:00-09:50

Contribution: Electronic transport in magnetic materials
Presenter: Christian Heiliger

09:50-10:40

Contribution: On the never-ending story of extracting effective tensorial spin Hamiltonians from ab initio
Presenter: Stefan Blügel

10:40-11:00
Coffee break

CHAIR: ANTONIO SANNA

11:00-11:50

Contribution: Proximity-Induced Superconductivity in Gd Layers on Nb: First-Principles Study with U term
Presenters: Balázs Újfalussy; Kyungwha Park

11:50-12:40

Contribution: Multiorbital Pairing Effects in Superconductors from First Principles
Presenter: Gábor Csire

12:40-14:00

Lunch break

Departure