Wannier 2022 Summer School

16 - 20 May 2022 An ICTP Hybrid Meeting Trieste, Italy

This 5-day school consists of lectures and hands-on sessions on a wide range of electronic-structure methods based on Wannier functions. The event targets graduate students, early-career scientists and experienced users.

Description:

Wannier functions (WFs) are used to understand the nature of chemical bonding, calculate topological and geometrical quantities, efficiently interpolate bandstructure properties and more. This event includes highlight talks that provide a historical and broad perspective on WFs in electronic structure, dedicated lectures to the theory and methods of WFs, as well as hands-on tutorials at the basic and advanced level. The school is designed to allow participants to join both in-person and online, and covers a wide range of complex materials properties using several software packages.

Topics:

- Maximally-localized Wannier functions (Wannier90)
- Advanced Wannier functions methods: symmetry-adapted, SCDM, transport (Wannier90)
- Partly occupied Wannier functions (ASE)
- Tight-binding models (PythTB)
- Topological properties (Z2pack & WannierTools)
- Berry-phase properties (WannierBerri)
- Automated wannierisation (AiiDA)
- Electron-phonon coupling (EPW)
- Dynamical mean-field theory (TRIQS)

In person participation: As regards the COVID-19 policy, we advise to follow the updated rules available on the ICTP page <u>Access Guidelines for Visitors</u>.



Further information: http://indico.ictp.it/event/9789/ smr3705@ictp.it

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Local Organiser:

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Speakers:

R. ARITA, Tokyo University and RIKEN, Japan S. BECK, Flatiron Institute, USA F. GIUSTINO, UT Austin, USA L. LIN, UC Berkeley, USA N. MARZARI, EPFL, Switzerland A. MOSTOFI, Imperial College London, UK Y. NOMURA, Keio University, Japan S. PONCÉ, EPL, Belgium J. QIAO, EPFL, Switzerland R. RESTA, CNR-IOM, Italy I. SOUZA, CFM and UPV, Spain K. THYGESEN, DTU, Denmark D. VANDERBILT, Rutgers University, USA M. VERGNIORY, DIPC, Spain V. VITALE, Imperial College London, UK

The School will be followed the week after (23 - 27 May 2022) by the <u>Wannier 2022 Developers</u> <u>Meeting</u> (smr3757), devoted to foster integration between several packages composing the Wannier software ecosystem.

Q. WU, IOPCAS, China

J. YATES, Oxford University, UK

Deadline:

20 March 2022

Trieste, Ital



Online application: http://indico.ictp.it/event/9789/

Female scientists are encouraged to apply.



A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.







The Abdus Salam International Centre for Theoretical Physics

