Abinit school on ground state, linear response properties and dynamics

Prague, 2–6 September 2019

LIÈGE université

FACULTY OF NUCLEAR SCIENCES AND PHYSICAL ENGINEERING CTU IN PRAGUE

FZU Institute of Physics of the Czech Academy of Sciences

Website
http://palata.fzu.cz/abinitschool

Venue Prague, Czech Republic

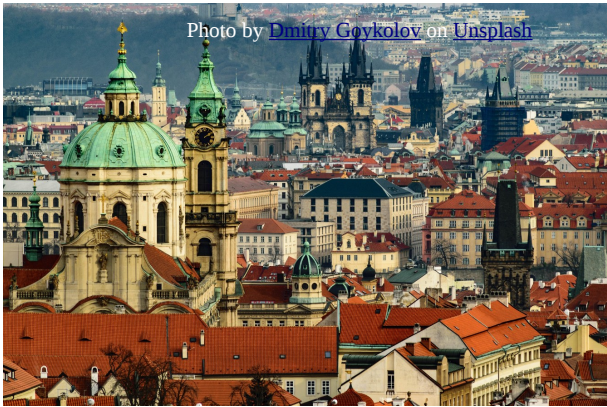
Abinit is a software suite to calculate the optical, mechanical, vibrational, and other observable properties of materials. Starting from the quantum equations of **density functional theory**, you can build up to advanced applications with **perturbation theories** based on DFT, and **many-body Green's functions** (GW and DMFT).

Organizers Eric Bousquet (University of Liège), Sabine Körbel (Trinity College Dublin), Ladislav Kalvoda (Czech Technical University), Marek Paściak, Pavel Márton, Jiří Hlinka (Institute of Physics of the Czech Academy of Sciences)

Sponsors Psi-k Network, Czech Technical University, Institute of Physics of the Czech Academy of Sciences, University of Liège

Scope of the school

- **Ground state properties**
- **M**olecular **D**ynamics, **P**ath-**I**ntegral **MD**, **N**udged-**E**lastic-**B**and calc.
- **Linear response** (DFPT) for phonons, Born/magnetic effective charges, dielectric/elastic/piezoelectric/ magnetoelectric tensors, nonlinear electro-optical coefficients, Raman intensities, magnetic susceptibility
- Berry phase calculation of the **polarization**
- **Applied** E, D and B **field**
- **Post-processing** (Abipy, Agate), analysis of displacive **phase transitions**
- **Second-principles** Multibinit code for simulations of large cells with temperature effects and dynamics
- **Parallel** & highly parallel implementations of Abinit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