

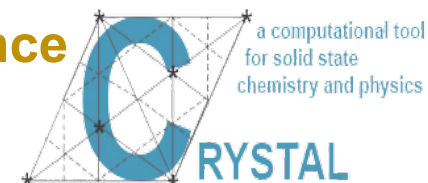


CRYSTAL – DFT Modelling in Nanoscience

In-person workshop with Hands-on Training

Feb 13-16, 2023

Venue: A43, INST Mohali



13 February

Opening Session

10:00-10:10 hr	Prof. Abir De Sarkar (Dean, Faculty) , INST, India
10:10-10:15 hr	Prof. Amitava Patra (Director, INST), India
10:15-10:20 hr	Prof. Ravi Pandey, Michigan Technological University, USA

Session-1 (Chair: Prof. Ravi Pandey)

10:20-11:00 hr	Prof. Amitava Patra, INST, India (<i>Experiment and Theory -Modelling</i>)
11:00-11:40 hr	Prof. Silvia Casassa, University of Torino, Italy (<i>Symmetry, Periodicity & SCF</i>)

Coffee Break: 11:40-12:00 hr

Session-2 (Chair: Prof. Silvia Casassa)

12:00-12:40 hr	Dr. Lorenzo Dona, University of Torino, Italy (<i>Hamiltonian, DFT functionals and dispersive corrections</i>)
12:40-13:20 hr	Prof. Bartolomeo Civalleri, University of Torino (<i>How to work with localized atomic orbital basis set</i>)

Lunch Break: 13:20-14:30 hr

Session-3: Hands-on Training I

14:30-16:30 hr	Input/Output
	Geometry Input & Manipulations
	Visualization
Coffee Break: 16:30-17:00 hr	
17:00-18:30 hr	Basis Set Hamiltonian Energy

14 February

Session-1 (Chair: Prof. Ehesan Ali)

09:40-10:20 hr	Prof. Bartolomeo Civalleri, University of Torino, Italy (<i>How to deal with unpair electrons: spin-density and Magnetic systems</i>)
10:20-11:00 hr	Prof. Silvia Casassa, University of Torino, Italy (<i>One-electron Properties (charge density & potential maps, band, DOS, COHP)</i>)
11:00-11:40 hr	Dr. Chiara Ribaldone, University of Torino (<i>Geometry Optimization & Equation of States</i>)

Coffee Break: 11:40-12:00 hr

Session-2 (Chair: Dr. Chandan Bera)

12:00-12:40 hr	Prof. Silvia Casassa, University of Torino, Italy (<i>Electron density analysis (Compton profile, Bader)</i>)
12:40-13:20 hr	Dr. Chiara Ribaldone, University of Torino, Italy (<i>Frequencies & Spectra (IR + Raman)</i>)

Lunch Break: 13:20-14:30 hr

Session 3: Hands-on Training II

14:30-16:30 hr	Geometry Optimization
	How to compute & Visualize IR and Raman Spectra
	Equation of States
Coffee Break: 16:30-17:00 hr	
17:00-18:30 hr	One-electron properties: Band Structure/DOS/Charge Density



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15 February

Session-1 (Chair: Prof. Puru Jena)

9:40-10:20 hr	Prof. Bartolomeo Civalleri, University of Torino, Italy (How to model defects and low-dimensional systems)
10:20-11:00 hr	Prof. Abir De Sarkar, INST, India (Energy conversion in Low-dimensional systems)
11:00-11:40 hr	Prof. Ravi Pandey, Michigan Technological University, USA (Optical properties of materials)

Coffee Break: 11:40-12:00 hr

Session-2 (Chair: Dr. Ashok Kumar)

12:00-12:40 hr	Dr. Chiara Ribaldone, University of Torino, Italy (From phonon to thermodynamics ...till MD!)
12:40-13:20 hr	Prof. Silvia Casassa, University of Torino, Italy (Electron transport in CRYSTAL (Seebeck, electron conductivity, power factor))

Lunch Break: 13:20-14:30 hr

Session-3: Hands-on Training III

14:30-15:30 hr	Electron transport and thermodynamics
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Excursion: 15:30-18:30 hr

Dinner: 19:30 hr onwards

16 February

Session-1 (Chair: Prof. Bartolomeo Civalleri)

09:40-10:20 hr	Dr. Lorenzo Dona, University of Torino, Italy (Tackling size and structural complexity with CRYSTAL: MOFs as a case study)
10:20-11:00 hr	Prof. Suneeta Srivastava, Panjab University & Central University of Haryana, India (Photocatalytic applications)
11:00-11:40 hr	Prof. Ashok Kumar, Central University of Punjab, Bhatinda, India (Machine learning)

Coffee Break: 11:40-12:00 hr

Session-2/Special Session (Chair: Prof. Abir De Sarkar)

12:00-12:40 hr	Prof. Puru Jena, Virginia Commonwealth University, USA (From clusters to crystals: a journey)
12:40-13:20 hr	Prof. Rajeev Ahuja, IIT Ropar & Uppsala University, Sweden (Future of computing in India)

Lunch Break: 13:20-14:30 hr

Session 3: Hands-on Training IV

14:30-16:00 hr	Surfaces and defects modeling
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Coffee Break: 16:00-16:30 hr

Closing Session

16:30-17:00 hr	Vote of thanks
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