## International Workshop & NIS colloquium

# Recent advances in developing computational tools for solid state calculations

**Tuesday 19th December 2023 - Aula Diagonale**

**Department of Chemistry (Via P. Giuria 7 - 10125 Turin, Italy)**

**Organizers:** Silvia Casassa, Bartolomeo Civalleri, Jacques K. Desmarais, Alessandro Erba

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| 14:00 | *OPENING REMARKS - Organizers* |
| | **Alessandro ERBA** - Chairperson - Department of Chemistry and NIS, University of Torino |
| 14:10 | **Jean-Pierre FLAMENT** Department of Physics, University of Lille (FR)<br>***The Davidson's diagonalization in CRYSTAL*** |
| 14:40 | **Davide MITOLI** Department of Chemistry and NIS, University of Torino<br>***Anharmonicity in lattice dynamics and vibrational spectroscopies: recent developments in CRYSTAL*** |
| 15:00 | **Chiara RIBALDONE** Department of Chemistry and NIS, University of Torino<br>***Ab initio Born-Oppenheimer molecular dynamics in the CRYSTAL code*** |
| 15:20 | **Naiara MARANA** Department of Chemistry and NIS, University of Torino<br>***Modeling and characterization of multiwall nanotubes with CRYSTAL program*** |
| 15:40 | **Eleonora ASCRIZZI** Department of Chemistry and NIS, University of Torino<br>***CRYSTALpytools: a new Python framework for the CRYSTAL code*** |
| *16:00* | *Coffee break* |
| | **Silvia CASASSA** - Chairperson - Department of Chemistry and NIS, University of Torino |
| 16:30 | **Stefano PITTALIS** CNR-Nanoscience, Modena<br>***Gauge theory of density functionals: from first principles to practical approximations for non-collinear magnetism*** |
| 17:00 | **Jacques K. Desmarais** Department of Chemistry, University of Torino<br>***Recent progress in the treatment of magnetic fields in the CRYSTAL Code*** |
| 17:20 | **Lorenzo DONÀ** Department of Chemistry and NIS, University of Torino<br>***Simplified electronic structure methods for solid state calculations with CRYSTAL: development and applications*** |
| 17:40 | **Giacomo AMBROGIO** Department of Chemistry and NIS, University of Torino<br>***GPU acceleration of linear algebra in the CRYSTAL Code*** |