



Important: The number of participants is limited to approx. 25 and the pre-registration is required.

- **Preregistrations deadline is March 21, 2016 (see below for details)**

Place : vacation center, mediterranean seashore →

Dates 19 – 23 September 2016



– **First circular** –

→ **General information**

This five-day course will cover key aspects of lattice and molecular dynamics simulation techniques with a particular emphasis on modelling dynamical properties of materials. The school will consist of lectures from subject experts, presenting the underlying models and basics of the methods; these theoretical presentations will be complemented with practical sessions.

Poster and oral sessions for presentations by participants will also be organised.

The main objective of the school is to provide information that will allow the attendees to become independent and conscious users of the lattice or molecular dynamics simulations in their own research.

→ **Participants : who should attend ?**

The school is aimed at researchers of all levels working in the field of solid state and chemical physics, physical chemistry, and materials science, and willing to benefit from the use of atomistic simulation techniques in their own studies. Postgraduate students being interested to attend are welcome. Participation of academics and industry researchers is also encouraged.

Prerequisites: although the knowledge of solid state physics, crystallochemistry, optics and electricity at the graduate university level are a prerequisite, the lectures will include an introductory part covering the basics necessary for following the course. Moreover a list of recommended readings will be communicated in advance. To follow the practical sessions the participants will have to bring their own computer. There is no special requirement to OS used (Windows, iOS, Linux) ; the practical sessions will simultaneously be shown using a videoprojector, allowing you to follow in case of failure of your PC.



Course objectives and program

The objectives of the school is mainly to allow participants to become autonomous for implementing lattice or molecular dynamics simulations in their own studies. Participants will thus receive all tools both theoretical and practical, including software, that will allow them to follow practical exercises during the school, and to treat simulation problems by themselves after the school.

Participants will also have the possibility to present their research work and problems to be simulated, in short talks or poster sessions.

The program covers Lattice Dynamics (LD) and Molecular Dynamics (MD) – two computer simulation techniques. Their similarities and differences. Backgrounds and approximations. Overview of effective interaction potentials. Variety of implementations. Some recent applications. Basic of MD. Specific details. MD results and material properties. Basic of LD. Specific details. LD results and material properties. LD package. Structure, synopsis, realizations, training. Example: crystal structure, phonons, elastic and piezoelectric constants, IR and Raman spectra of particular materials. MD package. Structure, synopsis, realizations, training. Example: same properties of the same crystals. Temperature impact. Phase transitions. Advanced LD methods. Beyond harmonic approximation. Phase transitions and soft modes. Framework structures and Rigid Unit Modes. LO-TO splitting and ferroelectrics. Advanced MD methods. Beyond micro-canonic ensemble. Non-equilibrium MD. Ab initio MD.



Organizing, and scientific committees

Scientific committee:

Mikhail SMIRNOV, Professor, Faculty of Physics, St Petersburg State University, Petrodvoretz, 194508 St Petersburg, Russia
smirnomb@rambler.ru

Konstantin SMIRNOV, Research Scientist, Laboratory of IR and Raman Spectrochemistry, CNRS – University Lille 1, 59655 Villeneuve d'Ascq, France
Konstantin.Smirnov@univ-lille1.fr

Aleksandr N. VTYURIN, Kirensky Institute of Physics, Russian Academy of Sciences, Siberian Branch, Russia
vturin@iph.krasn.ru

Dmitry CHERNYSHOV, Dr, Beamline Scientist (BM1A), SNBL/ESRF, CS40220, 38043 Grenoble CEDEX 9, France
dmitry.chernyshov@esrf.fr

Organizing committee:

Pierre SAINT-GRÉGOIRE, Professor, Universities of Nîmes and Toulon, MIPA Laboratory CS13019, 30021 NÎMES cédex, France
pstgregoire@gmail.com

Belkacem ZEGHMATI, Professor, University of Perpignan (UPVD), Laboratory LAMPS 52, Av. Paul Alduy, 66860 Perpignan cédex, France
zeghmati@univ-perp.fr

Yaovi GAGOU, University of Picardy (UPJV), Dr Hab, Associate professor, Laboratory LPMC 33, Rue St-Leu, 80039 Amiens cédex, France
yaovi.gagou@u-picardie.fr

Annie PÉREZ, University of Marseille, Dr Hab, Associate professor, IM2NP, Ecole Polytech' Marseille Technopôle de Château Gombert 13453 MARSEILLE Cedex 13, France
annie.perez@im2np.fr



Practical informations

The five-days school will be organized in a vacation center by the seaside (Mediterranean sea at 100 m) close to the French-Spanish border (closest airports Girona (Spain) served by low cost companies, and Perpignan (France) also served by train, TGV line Paris or Lille - Barcelona). Details will be given later on. Approximative fees, including the registration to the school, materials distributed at the school, and full pension in twin-rooms, will be about 800 € (accomodation + breakfast + lunch + dinner+ recreative activities) and 650 € for students (count +100€ for single room). A banquet will be organised. The fee for accompanying persons is 50 % of the normal fee, it includes the full-board accomodation + banquet + recreative activities ; we shall propose special discount for families if you desire to come with children, details on request.



Preregistration

Because for such a school the number of participants is limited in reason of the practice sessions, a preregistration is necessary in advance. The applications will be selected in the order of their arrival, and after the first 25 accepted applications, a waiting list will be established. You will be informed on the result (acceptation, waiting list, rejection) around march, 23.

Preregistrations will be closed on march, 21. They should be made by e-mail.

Consult regularly the pages of the school in the site of COLLABORATING ACADEMICS (<http://co-ac.com>) or follow in LinkedIn.

PREREGISTRATION FORM

deadline march, 21 (2016)

By e-mail to lamodyschool@co-ac.com, please fill, copy and paste the following:

Family name:

Given name:

Gender:

Age:

Institution:

Professional address (full address):

Town:

Country:

Professional e-mail:

Secondary e-mail:

Phone number (include international dialing code):

Functions/occupied position:

Field:

Last obtained diploma (nature and date):

Accompanying person (Yes/No)

Accompanying children (Yes/no), number and age

Motivation to attend the school (indicative):

Would you like to make a communication (annex abstract) (Yes/No, poster or oral)?

Special requirements (diet, etc.):

For students:

Name of supervisor:

e-mail address of supervisor:

Does your supervisor support your application to attend the school?

(For students, recommendation letter of supervisor should be sent, included or apart)



Important dates

Preregistration deadline: March, 21 – Detailed informations will be sent in the second circular on March, 23.

Dates of the school: 19 – 23 September 2016