

MODELLING SCHOOL IN CHEMISTRY, BIOLOGY, PHYSICS - 2021

Contacts :

Arnaud.Fihey@univ-rennes1.fr

Adele.laurent@univ-nantes.fr

All sessions will be held online.

Monday - 01/03

9h-12h - Online

Rémi Marchal (ISCR, Rennes)

“Unix - calculation centers”

Introduction to Unix language and scientific calculations environments, how to work on a local or national computation cluster,

(Course in English)

14h-17h - Online

Rémi Marchal (ISCR, Rennes)

“Coding with Python - Lecture”

Introduction to programming with Python language

(Course in English)

Tuesday - 02/03

9h-12h - Online

Rémi Marchal (ISCR, Rennes)

“Coding with Python - Practical session 1”

Introduction to programming with Python language

(Course in English)

14h-17h - Online

Rémi Marchal (ISCR, Rennes)

“Coding with Python - Practical session 2”

Introduction to programming with Python language

(Course in English)

Wednesday 03/03

9h-12h - Online

Florent Di Meo (IPPRITT, Limoges)

“Modeling biological systems - Lecture”

Molecular dynamics simulations, Biological systems, Force field, Enhanced sampling.

(Course in English)

14h-17h - Online

Florent Di Meo (IPPRITT, Limoges)

“Modeling biological systems - Practical session”

Practical examples of molecular dynamics and sampling methods.

(Course in English)

Thursday 04/03

9h-12h - Online

Maximilien Levesque (Aqemia)

Benjamin Chantemargue (InsiliBio)

“Theoretical chemistry in industry”

Applications of BioInformatics and Drug-design for research in industry.

(Course in French/English depending on the audience)

Friday 05/03

9h-12h - Online

Rémi Maurice (Subatech, Nantes)

“Molecular Quantum Chemistry - Lecture”

Principles of quantum chemistry, Hartree-Fock and post Hartree-Fock models, Density Functional Theory.

(Course in English)

14-17h - Online

Arnaud Fihey, Karine Costuas (ISCR, Rennes)

“Molecular Quantum Chemistry - Practical session”

Initiation to the Gaussian software - ground state properties of molecules

(Course in French/English depending on the audience)

Monday - 08/03

9h-12h - Online

Denis Jacquemin (CEISAM, Nantes)

“Excited-States in Molecules - Lecture”

Excited states, TD-DFT, second-order methods, modelling of optical spectra

(Course in English)

14h-17h - Online

Arnaud Fihey, Karine Costuas (ISCR, Rennes)

“Excited-States in Molecules – Practical session”

TD-DFT calculations with the Gaussian software – excited-state properties of molecules

(Course in French/English depending on the audience)

Tuesday - 09/03

9h-12h - Online

Frédéric Guégan (IC2MP, Poitiers)

“Conceptual DFT: A paradigm for understanding chemical reactivity and selectivity” - Lecture

First-principles prediction of reactivity and selectivity; chemical interaction theory; electron density based analyses.

(Course in French/English depending on the audience)

14-17h - Online

Frédéric Guégan (IC2MP, Poitiers)

“Hands on: Conceptual DFT” - Practical session

(Course in French/English depending on the audience)

Wednesday - 10/03

9h-12h - Online

François Lique (IPR, Rennes)

“Introduction to Astrochemistry - Lecture”

Modeling interstellar medium, stars formation, kinetic, molecules, scattering processes

(Course in English)

14h-17h - Online

Boris Le Guennic (ISCR, Rennes)

“Modeling Lanthanides-based compounds - Lecture”

Magnetic and (chir-)optical properties of lanthanide complexes through the prism of *ab initio* calculations.

(Course in English)

Thursday - 11/03

9h-12h - Online

Georges Volonakis (ISCR, Rennes)

“Solid state quantum chemistry -Lecture”

Electronic structure of solids, Band structures, periodic, periodic DFT.

(Course in English)

14h-17h - Online

Georges Volonakis, Bruno Cucco (ISCR, Rennes)

“Solid state quantum chemistry -Practical session”

Periodic DFT calculations with the VASP software.

(Course in English)

Friday - 12/03

9h-12h - Online

Xavier Rocquefelte (ISCR, Rennes)

“Properties in solids - Lecture”

Magnetic properties in solid state.

(Course in French/English depending on the audience)

14h-17h - Online

William Lafargue-Dit-Hauret (IMN, Nantes)

“Properties in solids -Practical session”

Calculation of magnetic properties in solids with the VASP software.

(Course in French/English depending on the audience)