



POM-BASICS Summer School

**“Polyoxometalate Chemistry for
Fundamentals and Applications”**

La Rochelle-France, June 13-15th 2022



Session 3- Structural characterization and modelling

Part-2. Multiscale structural characterization techniques and modelling in POM chemistry

Trainer: Carles Bo, (Tarragone, Spain)



Abstract of the course:

The second part of the session will highlight the contributions of theoretical and computational methods to POMs chemistry. In the last two decades electronic structure studies and molecular dynamics simulations complemented the experimental techniques nicely. In addition to a brief overview of the theoretical methods and their recent evolution, we will discuss how the properties that can be derived from modelling (structural, electronic, spectroscopic, in solution) help solving several problems encountered experimentally and provide new insight as well.