Detailed Program of the School

Monday 24th June

8.30-9.00 *Arrival and registration*

9.00-10.00 **Introductory lecture: Basics of Vibrational Spectroscopy**
Boriana Mihailova (*Professor of Crystallography, Universität Hamburg*)
- Atomic dynamics of solids in a nutshell: phonons in crystals and vibrational density of state in glasses.
- Light-solid interaction processes: Raman scattering vs infrared absorption.
- The importance of symmetry: selection rules (showcase using the Bilbao crystallographic server) and polarized Raman / infrared spectra.
- How to collect a good-quality Raman spectrum

10.00-11.00 **Symmetry classification of the Raman signals and selection rules**
Mauro Prencipe (*Associate professor, University of Turin*)
Vibrational modes can be classified according to the irreducible representations of the point group to which the crystal or the molecule belongs. The symmetry properties of each vibrational mode determine the activity of the mode itself in response to the perturbation caused by the electromagnetic radiation interacting with it. Based on a symmetry analysis it is therefore possible to predict which modes are Raman-active, and under which polarization conditions

11.00-11.30 *Coffee break*

11.30-12.30 **Effect of composition on Raman scattering**
Boriana Mihailova (*Professor of Crystallography, Universität Hamburg*)
- The concept of one-mode / two-mode behavior
- Rock-forming silicates: showcases on nominally anhydrous and hydrous minerals
- Alkali silicate glasses.

12.30-13.30 *Lunch break*

13.30-14.30 **Effect of temperature and pressure on Raman scattering**
Boriana Mihailova (*Professor of Crystallography, Universität Hamburg*)
- Temperature dependence of atomic dynamics: Raman-peak positions, widths and intensities as a function of temperature.
- Pressure dependence of atomic dynamics: Raman-peak positions, widths and intensities as a function of pressure
- Phase transitions: soft-mode and hard-mode spectroscopy. Showcases of temperature-/pressure-induced phenomena in geomaterials.
- A note on second-order photon-phonon interactions as well as on resonance Raman scattering and why geoscientists should be aware of such processes.

14.30-15.30 **Raman spectroscopy by ab initio calculations**
Mara Murri (*Researcher, Department of Earth and Environmental Sciences, University of Pavia*)
How to calculate a Raman spectrum by HF/DFT calculations. Comparisons with experimental data. Theoretical experiments and applications in the framework of geological studies.

15.30-16.30 **From lattice dynamics to thermodynamics: a first principles approach**
Donato Belmonte (*Associate Professor, DISTAV, University of Genova*)
Micro to macro: from lattice dynamics to thermodynamic properties of crystalline solids. Basic principles of statistical thermodynamics: partition function and phonon density of states. Vibrationally-constrained thermodynamic predictive models: history (Einstein, Debye, Kieffer) and modernity (ab initio).

Tuesday 25th June

9.00-10.00 **Raman spectroscopy: Better do it right!**
Lutz Nasdala (*Professor for Mineralogy and Spectroscopy, Institute for Mineralogy and Crystallography, University of Vienna*)

The generally increasing interest in using Raman is in harsh contrast to the existing lack of training opportunities. As a result, a significant fraction of published "results" are tainted with uncertainty. The lecture attempts to summarise potential experimental artefacts and common mistakes, and to give hints on how to do proper analysis.

10.00-11.00 **Application of Raman and photoluminescence spectroscopy in gemstone analysis**
Lutz Nasdala (*Professor for Mineralogy and Spectroscopy, Institute for Mineralogy and Crystallography, University of Vienna*)
Both Raman spectroscopy, and the virtually omnipresent "enemy" laser-induced photoluminescence, have various applications in identifying and characterising gemstones. Examples include gem tourmaline, the historical Schneckenstein topaz, and gems in the Imperial Crown of the Holy Roman Empire.

11.00-11.30 *Coffee break*

11.30-12.30 **Raman elastic geothermobarometry of quartz and zircon inclusions in garnet**
Dr. Mattia Gilio (*Von Humboldt Research fellow*, Universität *Hamburg*)
Elastic geothermobarometry allows to interpret the conditions of mineral formation in metamorphic rocks from the difference in physical properties between a mineral inclusion and its surrounding host phase. This seminar deals with the basic theory of Raman-based elastic geothermobarometry and its application on quartz and zircon inclusion in garnet, from the initial measurement to the final P-T estimate.

12.30-13.30 *Lunch break*

13.30-14.30 **Raman spectroscopy applied to host-inclusion systems: a probe for in situ mineral rheology at non-ambient conditions**.
Nicola Campomenosi (*Researcher, Department of earth sciences, environment and life, University of Genoa*)
The contrast in the thermoelastic properties between a mineral inclusion and its host leads to residual stresses in the inclusion that change in magnitude and sign as function of different external pressure and temperature conditions. The seminar deals with showing how Raman spectroscopy can be used to quantify residual strain and stress in mineral inclusions at non-ambient conditions and how these data can be used to determine in situ the rheology of minerals undergoing different stress states.

14.30-15.30 **Raman spectroscopy and melt inclusions in metamorphic rocks**
Silvio Ferrero (*Associate Professor, University of Cagliari*)
Micrometric melt inclusions in high grade metamorphic rocks tell us the history of the chemical differentiation of the crust through time, and Raman spectroscopy is one of the main tools to rapidly extract reliable information from these tiny objects. We will see examples of how Raman spectroscopy allows us to clarify volatile budgets at depth, find new minerals and new magmatic processes, and understand the origin of peculiar polymorphs of feldspar – the data we need to correctly assess continental subduction and orogenetic processes.

15.30-16.30 Poster and talks by students

Wednesday 26th June

9.00-11.00 **Fluid inclusions**
Maria Luce Frezzotti (*Professor of Petrology, University of Milano Bicocca*)

11.00-11.30 *Coffee break*

11.30-12.30 **Raman spectroscopy and Machine Learning for thermal maturity assessment**
Natalia Amanda Vergara Sassarini (*Research fellow in Planetary Geology at CISAS, University of Padua*)
We will discuss the role of Raman spectroscopy in assessing the thermal maturity of source rocks. Additionally, we will explore how applying Machine learning on Raman spectra can facilitate maceral

recognition, aiding thermal maturity assessment of source rocks characterized by complex organic matter assemblages.

12.30-13.30 *Lunch break*

13.30-14.30 **Raman spectroscopy and mapping: from Earth and planetary sciences to tribology, material sciences, and biology**

Bruno Reynard (*Directeur de Recherches CNRS, Laboratoire de Géologie de Lyon*)

Raman spectroscopy and mapping is developed in Earth sciences with the aim of characterizing complex materials potentially submitted to extreme environments. This specificity finds applications in many other fields of science, and I show examples of transfer of know-how to various fields based on our work in Lyon

14.30-15.30 **Raman Spectroscopy of Carbonaceous Material: RSCM thermometry and more**

Olivier Beyssac (*CNRS senior scientist at IMPMC Paris (CNRS/Sorbonne Université/MNHN Paris, France*)

- The Raman spectrum of carbonaceous material: basics,
- How to measure the Raman spectrum of carbonaceous material,
- RSCM thermometry: how it works, successes and challenges,
- RSCM thermometry: some applications,
- Other applications.

15.30-16.30 Poster and talks by students

19.00-22.00 *School dinner*

Thursday 27th June

9.00-10.00 **Spectroscopy on Mars: what's up on the Red Planet?**

Olivier Beyssac (*CNRS senior scientist at IMPMC Paris* (*CNRS/Sorbonne Université/MNHN Paris*))

- Quick presentation of the NASA Mars2020 mission and Perseverance rover,
- Scientific instruments and techniques onboard Perseverance: Raman, LIBS, XRF and VISIR reflectance spectroscopy,
- A focus on time-resolved Raman spectroscopy (SuperCam instrument),
- Some scientific results obtained by Perseverance.

10.00-11.00 **Vibrational spectroscopy as a tool to characterize silicate glasses.**

Alessandro Pisello (*Post-doct research fellow, University of Perugia*)

- Silicate glasses theory and occurrence on Earth and terrestrial bodies.
- Disordered structures, short-range order, tetrahedral networks, Q speciation.
- Quantifying Q speciation with vibrational spectroscopy on synthetic glasses (simple compositions)
- Linking spectral features to chemical composition, iron speciation and water content for natural glasses: possibilities and limits.

11.00-11.30 *Coffee break*

11.30-12.30 **Raman Crystal Hunter software: application to mineral inclusions in diamonds**

Fabrizio Nestola (*Professor for Mineralogy, University of Padua*)

Natural diamonds are the only geological materials capable to preserve fragments of very deep Earth from about 120 to even 1000 km depth through its mineral inclusions. The deepest diamonds are named “super-deep diamonds” (also called sublithospheric diamonds) and are the most intriguing and likely most important diamonds to retrieve geological information on the deepest regions of our planet. Micro Raman spectroscopy is likely the most efficient technique in diamond research to investigate such tiny inclusions. We developed RamanCrystalHunter, a new software program designed to pre-process, analyse and identify Raman spectra by comparison with spectra in the RamanCrystalHunter Database. Here I will show how to use Raman Crystal Hunter software to obtain geobarometric information on super-deep diamonds.

12.30-13.30 *Lunch break*

13.30-14.30 **Elasticity of minerals in the deep interior of planets as determined by Brillouin scattering measurements**

Tiziana Boffa-Ballaran (*senior scientist, the Bayerisches geoinstitut*)

I will introduce the principles of Brillouin scattering and its role in determining mineral elasticity at high-pressure and high-temperature. Example will be given on how the elasticity of minerals coupled with seismic observations can be used to constrain the composition and mineralogy of planetary interiors.

14:30-17:30 **Practical parallel sessions**

Practical session (data collection on mineral, inclusions, on fluid inclusion, carbonaceous materials, "bring your own sample", tutorial on data collection and data processing).

Friday 28th June

9.00-10.00 **Practical sessions I**

From lattice dynamics to thermodynamics: a first principles approach (hands-on tutorial and practicals.

Donato Belmonte (*Associate Professor, DISTAV, University of Genova*)

Computational thermodynamics for phase equilibrium calculations at high pressure and temperature: application to mineral reactions and phase diagrams at planetary interior conditions. Practicals and hands-on tutorial on Gibbs free energy minimization method by in-house computer codes.

10.00-11.00 **Practical sessions II**

From lattice dynamics to Equations of State: a simplified approach

Ross J. Angel (Research Scientist, C.N.R. Instituto di Geoscienze e Georisorse, Padova, Italy)

The phonon density of states (pDOS) is responsible for the heat capacity and thermal pressure of solids, but is too complex to introduce into practical equations of state. This lecture will introduce and justify the simplified models for pDOS that can be used in PVT EoS.

11.00-11.30 *Coffee break*

11.30-12.30 Roundtable and Closing remarks

12.30-13.30 *Lunch break*