Pressure and Temperature: “natural” variables

**WHY** study matter under extreme pressures?

- Because the physicochemical properties of matter drastically change with the interatomic distances and the atomic spatial distribution.
- In fact, atmospheric-pressure conditions are almost the exception in most natural phenomena.
Pressure and Temperature: “natural” variables

**HOW** study matter under extreme pressures?

- **EXPERIMENTAL TECHNIQUES**
  - MACROSCOPIC
  - MICROSCOPIC

- **THEORETICAL MODELS**
  - PHYSICAL PHENOMENA
    - Structure
    - Phase Transitions
  - CHEMICAL PHENOMENA
    - Chemical Bond
    - Reactivity

Condensed Matter under Extreme Pressure and Temperature Conditions
# High Pressure Science & Technology

Multidisciplinary & Interdisciplinary

## General Programme

### Friday 28th

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16:30</td>
<td>Introduction. General Aspects</td>
<td>Valentin. G. Baonia, Universidad Complutense de Madrid, Spain</td>
</tr>
<tr>
<td>17:15</td>
<td>Theory &amp; Simulations I</td>
<td>Miriam Marqués, Universidad de Valladolid, Spain</td>
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<td></td>
<td>Coffee break (15 minutes)</td>
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</tr>
<tr>
<td>18:15</td>
<td>Theory &amp; Simulations II</td>
<td>Julia Contreras, Université Pierre et Marie Curie, France</td>
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### Saturday 29th

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<tbody>
<tr>
<td>10:00</td>
<td>High Pressure Techniques</td>
<td>Konstantin V. Kamenev, University of Edinburgh, UK</td>
</tr>
<tr>
<td>10:45</td>
<td>Pressure Scales</td>
<td>Stefan Kloz, Université Pierre et Marie Curie, France</td>
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<td></td>
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</tr>
<tr>
<td>12:00</td>
<td>Structural Determination</td>
<td>Julio Pellicer, Universidad de Valencia, Spain</td>
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<tr>
<td>12:45</td>
<td>Optical Spectroscopy</td>
<td>Fernando Rodríguez, Universidad de Cantabria, Spain</td>
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<td>Vibrational Spectroscopy</td>
<td>Alfonso San Miguel, Université de Lyon 1, France</td>
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<td>Chemistry at High Pressure</td>
<td>Margherita Citroni, LENS, University degli Studi di Firenze, Italy</td>
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### Sunday 30th

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<td>Geosciences &amp; Mineralogy</td>
<td>Maurizio Mattei, Instituto de Geosciencias IGE, Spain</td>
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<tr>
<td>10:45</td>
<td>Biosciences</td>
<td>Roland Winter, Technische Universität Dortmund, Germany</td>
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<td>Food Science &amp; Technology</td>
<td>David Flores, Hiperbaric S.A., Burgos, Spain</td>
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<td>12:45</td>
<td>Challenges &amp; Hot Topics</td>
<td>John Tse, University of Saskatchewan, Canada</td>
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<td>13:30</td>
<td>Exams &amp; Handing of Certificates</td>
<td>J. Manuel Recio, Universidad de Oviedo, Spain</td>
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Friday afternoon; Saturday morning; Saturday afternoon; Sunday morning; T: Theory; E: Experiments; A: Applications
High Pressure Science & Technology

Multidisciplinary & Interdisciplinary

Joint AIRAPT-25 & EHPRG-53
International Conference On High Pressure Science And Technology


2. Food Science and Technology (Food Microbiology, Food Engineering, High Hydrostatic Pressure Processing, High Pressure Thermal Sterilization, Ultra-High Pressure Homogenization)

3. Metrology and Industrial Applications (Pressure Scales, Polymorphism and Polymorphism in Medical and Pharmaceutical Applications, Biotechnological and Cosmetic Applications)

4. Theory (Modelling and Simulation, New Techniques and Methods)


6. Condensed Matter I (Equations of State, Phase Transitions, Melting, Thermophysical Properties)

7. Condensed Matter II (Electronic, Magnetic and Transport Phenomena, Superconductivity, Strongly Correlated Systems)

8. Dynamical Pressure (Dynamical Response of Materials, Shock Wave Techniques)


10. Nanoscience and Nanotechnology (Quantum Dots, Nanoparticles, Nanostructures, 1D and 2D Materials, Nanotubes, Graphene)


Introduction. General Aspects

High Pressure Science & Technology

Matter at High Pressure Program (2008-2015)

SCIENTIFIC GOALS

I. Water and life-related systems
   a. Synthesis, properties and stability of ice clathrates
   b. High pressure effects on aqueous solutions of supramolecular aggregates and proteins
   c. Microbiology under extreme conditions of pressure and temperature

II. Molecular systems: physical properties and chemical reactivity
   a. Pressure as a probe on unsaturated NOCH systems
   b. Pressure-induced reactivity on NOCH materials

III. Structure, stability, and reactivity of minerals
   a. Pressure-Temperature-Composition (PTx) diagrams and physical properties of: $\text{ABO}_3$ ($\text{AO-BO}_2$), $\text{ABO}_4$ ($\text{AO}_2$-$\text{BO}_2$) and $\text{AB}_2\text{O}_4$ ($\text{AO-BO}_2$) oxides
   b. Catalytic properties of minerals on abiotic organic synthesis

Condensed media PES
### Pressure Definition and Units

#### Common Pressure Units

<table>
<thead>
<tr>
<th>Unit</th>
<th>psi</th>
<th>atm</th>
<th>mm Hg</th>
<th>cm Hg</th>
<th>oz/in²</th>
<th>Kg/cm²</th>
<th>°Hg</th>
<th>mm Hg (torr)</th>
<th>cmHg</th>
<th>mbar</th>
<th>bar</th>
<th>Pa (N/m²)</th>
<th>kPa</th>
<th>MPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0361</td>
<td>1</td>
<td>25.4</td>
<td>17.36</td>
<td>0.0755</td>
<td>0.0054</td>
<td>0.0736</td>
<td>1.866</td>
<td>0.187</td>
<td>2.488</td>
<td>101.3</td>
<td>1.013</td>
<td>0.1013</td>
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<tr>
<td>14.7</td>
<td>1</td>
<td>1</td>
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<td>17.36</td>
<td>0.0755</td>
<td>0.0054</td>
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#### SI Units

\[ [P] = \left[ \frac{F}{S} \right] = N \cdot m^{-2} = kg \cdot m^{-1} \cdot s^{-2} = Pa \]
This determines -and often limits- the experimental techniques that can be employed (depending of the pressure range of interest) and the states in a potential energy surface that can be accessed and probed.

\[ P = \frac{F}{S} \leftrightarrow \frac{E}{V} \]

This determines -and often limits- the experimental techniques that can be employed (depending of the pressure range of interest) and the states in a potential energy surface that may be accessed and/or probed in a HP experiment.

PRESSURE
Structure.- Relative Orientations
Geometry.- Conformations, etc.
Electronic Structure

Ground State

**PRESSURE**
- Structure: Relative Orientations
- Geometry: Conformations, etc.
- Electronic Structure

New chemistry
- Different from solution of gas-phase
- No solvents, initiators or catalysts

**COMPRESSION**
- Pressure Induced Reactivity

- Ground State
- Excited States

**V. G. Baonza**

**PRESSURE**
- Structure: Relative Orientations
- Geometry: Conformations, etc.
- Electronic Structure

**THERMODYNAMICS**
\[
\left( \frac{\partial \ln K}{\partial P} \right)_T = - \frac{1}{RT} \sum_i V_i V_i^0 = - \frac{\Delta V^0}{RT}
\]

**EXAMPLE REACTION**
\[
2\text{AlCl}_3 + 2\text{Fe} + 3\text{H}_2\text{O} \rightarrow \text{Al}_2\text{O}_3 + 2\text{FeCl}_3 + 3\text{H}_2
\]

**VOLUME CHANGES**
- $V = 305\text{cm}^3$
- $V = 131\text{cm}^3$

**KINETICS**
\[
\left( \frac{\partial \ln k}{\partial P} \right)_T = - \frac{\Delta V^0}{RT}
\]
- Activation:
- Volume:

**COMPRESSION**

**Diagram:**
- Ground State
- Excited States
- Energy ($\Delta E$)
- Volume ($\Delta G$)

PRESSURE
Structure.- Relative Orientations
Geometry.- Conformations, etc.
Electronic Structure

TEMPERATURE
Structure.- Relative Orientations
Atomic movements (phonons/vibrations)
Excited States Mixing

Introduction. General Aspects

V. G. Baonza
Introduction. General Aspects


PRESSURE
- Structure: Relative Orientations
- Geometry: Conformations, etc.
- Electronic Structure

RADIATION
- Absorption creates reactive centers
- HP decreases excitation gap
- HP favors multiphotonic processes

Absorption creates reactive centers
HP decreases excitation gap
HP favors multiphotonic processes
High Pressure Techniques

Static Pressures

Dynamic Pressures
Some Historic Remarks in HP History

Percy W. Bridgman

Considered as the most outstanding HP researcher all-time:
- 50 years of HP studies (ca. 1910-†)
- Development of the first pressure scale (mercury resistance)
- He studied ca. 1000 substances/compounds under pressure
- Discovering of new HP phases of ice
- Complete Collection of Thermodynamic Formulas (PR 3, 273, 1914)

"...It is well known that under ordinary conditions water is abnormal in many respects. The effect of high pressure is to wipe out this abnormality....

"...If the white of an egg is subjected to hydrostatic pressure at room temperature, it becomes coagulated, presenting an appearance much like that of a hard boiled egg.....The effect of temperature, which is not large, seems to be such that the ease of coagulation increases at low temperatures, contrary to what one might expect...."
J. Biol. Chem. 19 (1914) 51-512.
Some Historic Remarks in HP History

The Synthesis of Diamond

Tracy Hall & GE Team
Some Historic Remarks in HP History

The Synthesis of Diamond
Some Historic Remarks in HP History

The Diamond Anvil Cell (DAC) - 1958

Ice VI (0.96 GPa)

Charles E. Weir, Ellis R. Lippincott, and Elmer N. Bunting (NBS)

Alvil van Valkenburg
Some Illustrative DAC Experiments

Nitrogen at 1.3 Mbar (LLNL, 1996)
Some Illustrative DAC Experiments

Agl Phase Diagram

Water/Ices Phase Diagram

Ice Freezing
under 9.8 kbar of pressure
Hydrostatic vs. Non-Hydrostatic Experiments

Diamond Anvil Cell

Non-hydrostatic Compression

Hydrostatic Compression
Hydrostatic vs. Non-Hydrostatic Experiments

Diamond Anvil Cell

Non-hydrostatic Compression

Hydrostatic Compression
Hydrostatic vs. Non-Hydrostatic Experiments

Diamond Anvil Cell

Pressure Distribution

(a) Non-hydrostatic  (b) Hydrostatic

Non-hydrostatic Compression

Hydrostatic Compression
Hydrostatic vs. Non-Hydrostatic Experiments

UCM (2011)
### General Programme

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- **T2** Theory & Simulations I 17:15  Miriam Marqués, Universidad de Valladolid, Spain
  - Coffee break (15 minutes)
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- **E3** Structural Determination 12:00  Julio Pellicer, Universidad de Valencia, Spain
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- **Food Show** 14:15  Hiperbaric S.A.

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**Introduction. General Aspects**

**Summer Under Pressure School & Some Reference Books**
THANK YOU ... and enjoy!

Valentín García Baonza
MALTA-Consolider Team

SUPERS is associated with

Joint AIRAPT-25 & EHPRG-53
International Conference On High Pressure Science And Technology

August 28th-30th
Madrid, 2015