PROPOSAL
Syllabus

March 23, 2022

1) Name and surname

Dr Giorgio F. Signorini
Università di Firenze,
Dipartimento di Chimica

- CV (1-2 pag) + picture: see attachment
- Selected bibliometric data:
  - Scopus CITESCORE: 2012=6.7, 2014=8.8
  - WoS 5 year IF: 2012=3.702, 2014=5.76
- Selection of the 10 most relevant publications:

1. Giorgio F. Signorini, Pier Francesco Fracassi, Roberto Righini, and Raffaele Guido Della Valle. Energy decay mechanisms and anharmonic lattice dynamics: the case of solid nitrogen. Chem. Phys. , 100:315329, 1985
2. Giorgio F. Signorini, J.L. Barrat, and M.L. Klein. Structural relaxation and dynamical correlations in a molten salt near the liquid-glass transition: a molecular dynamics study. J. Chem. Phys. , 92:12941303, 1990
3. Giorgio F. Signorini, Roberto Righini, and Vincenzo Schettino. Lattice dynamics of the orthorhombic phase of KClO 4 : Ewald's method in molecular coordinates. Chem. Phys. , 154:245261, 1991
4. Raffaele Guido Della Valle, Giorgio F. Signorini, and Piero Procacci. Vibrational density of states and homogeneous linewidth in molecular crystals: many-phonon processes in nitrogen. Phys. Rev. B , 55:1485514864, 1997
5. Angela Zoppi, Giorgio F. Signorini, Luca Bachechi, and Franco Lucarelli. Characterization of painting materials from eritrea rock art sites with non-destructive spectroscopic techniques. Journal of Cultural Heritage , 3:299308, 2002
6. G. F. Signorini, Riccardo Chelli, Piero Procacci, and Vincenzo Schettino. Energetic fitness of histidine protonation states in PDB structures. Journal of Physical Chemistry B , 108:1225212257, 2004.
7. S. Marsili, Giorgio F. Signorini, R. Chelli, M. Marchi, and P. Procacci. Orac: A molecular dynamics simulation program to explore free energy surfaces in biomolecular systems at the atomistic level. J. Comput. Chem. , 31: 11061116, 2010. ISSN 0192-8651.
8. R. Chelli and Giorgio F. Signorini. Serial generalized ensemble simulations of biomolecules with self-consistent determination of weights. Journal of Chemical Theory and Computation, 8(3):830842, 2012.
9. Carlo Guardiani, Giorgio F. Signorini, Roberto Livi, Anna Maria Papini, and Piero Procacci. Conformational landscape of n-glycosylated peptides detecting autoantibodies in multiple sclerosis, revealed by hamiltonian replica exchange. The Journal of Physical Chemistry B , 116(18):54585467, 2012.

10. Giorgio F. Signorini, Edoardo Giovannelli, Yannick G. Spill, Michael Nilges, and Riccardo Chelli. Convective replica-exchange in ergodic regimes. Journal of Chemical Theory and Computation , 10(3):953958, 2014.

2) Title of the course:

STRUCTURE OF INORGANIC GLASSES

3) Course content detailed per lesson of 2 h

(time and place will be arranged with subscriber students)

1. Simple oxide glasses
2. Multi-component oxide glasses
3. Non-oxide glasses with CRN structure
4. Other non-oxide glasses (metal, ionic)

4) Course program (150-200 words)

Simple Oxide Glasses. SiO_2glass: comparison with known crystal structures, basic tetrahedral unit, experimental evidence (XRD, NS, Raman). Borate glasses: stability with respect to crystal forms, basic triangular unit and boroxol ring. Multicomponent oxide glasses. Alkali silicate glasses, structural effect of the addition of the alkali metal, average number of shared vertices; Q^n species and their dependence on molar fraction of alkali oxide, bond model; alkali/alkaline earth silicate glasses. Alkali borate glasses, structural effect of the addition of the alkali oxide, the boron anomaly, B^n species and bond model for alkali borate glasses. Phosphate glasses. Glasses with multiple glass-formers and glass-modifiers: alkali borosilicate glasses, alkali aluminosilicate glasses. Non-oxide CRN glasses. Amorphous silicon and germanium, excess of constraints. Chalcogenide glasses: bond model for a generic$A_x^{III}B_{1-x}^{II}$ compound, complete chemical order, random covalent network, thermodinamical-statistical model. Metal glasses. Binary compounds, RCP model with and without structure relaxation, chemical order and local structure in T-M glasses, efficient cluster packing model, Voronoi analysis. Discrete anion glasses. Structure and its relaxation.

5) Suggested reading

- A. K. Varshneya. Fundamentals of Inorganic Glasses. Academic Press, 1994. ISBN 0-12-714970-8.

- J. E. Shelby. Introduction to Glass Science and Technology, 2nd edition. The Royal Society of Chemistry, 2005. ISBN 0-85404-639-9.
- Giorgio F. Signorini, Structural Properties of Glasses: an Introduction (lecture notes), chapters 1-3, http://www1.chim.unifi.it/u/signo/did/glass-structure/glass_structure.pdf

6) Learning Objectives

Understanding the structures of different classes of glasses on the basis of established models (CRN, RCP, other) examined in the first module of this course.

7) Knowledge and skills to be acquired

(see previous point)

8) Prerequisites

- First module of this course, see "lecture notes" in "Suggested Reading" above. Attendance of this past module is not strictly required, as long as the student has read and understood the lecture notes.

9) Teaching Methods

Traditional and/or online lessons, 4x2h

10) Further information

None

11) Type of Assessment:

Written test: the student will be assigned a recent paper on the subject of the course and will have to write a short essay (1-2 pages) about it.

The final evaluations will have to be validated within 1 month of the end of the course.

Total hours: 8h frontal lessons (3 ECTS)

Period: The lessons will be delivered online or both online and in presence. The lessons will be recorded and available to all the students that cannot take part to the lessons in streaming. The Webex platform will be used