Atomistic Modeling of Glass Structure & Glass Properties

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OVERVIEW

Materials are essentials for our way of life

- We use materials to create tools or objects

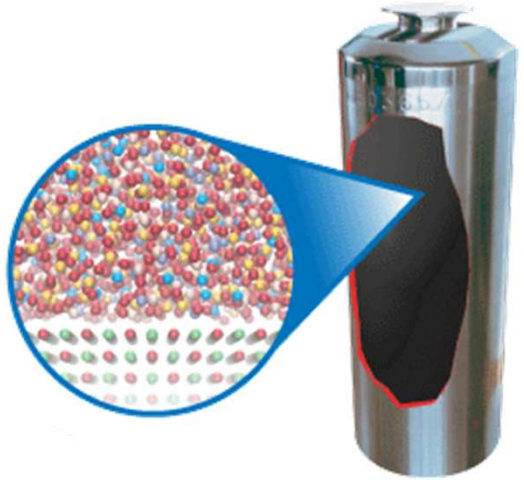
- Materials science « triangle »

  Synthesis – structure – properties

- We need glass because it is transparent and strong

  windows, containers, lighting, optics

Glass everywhere ?

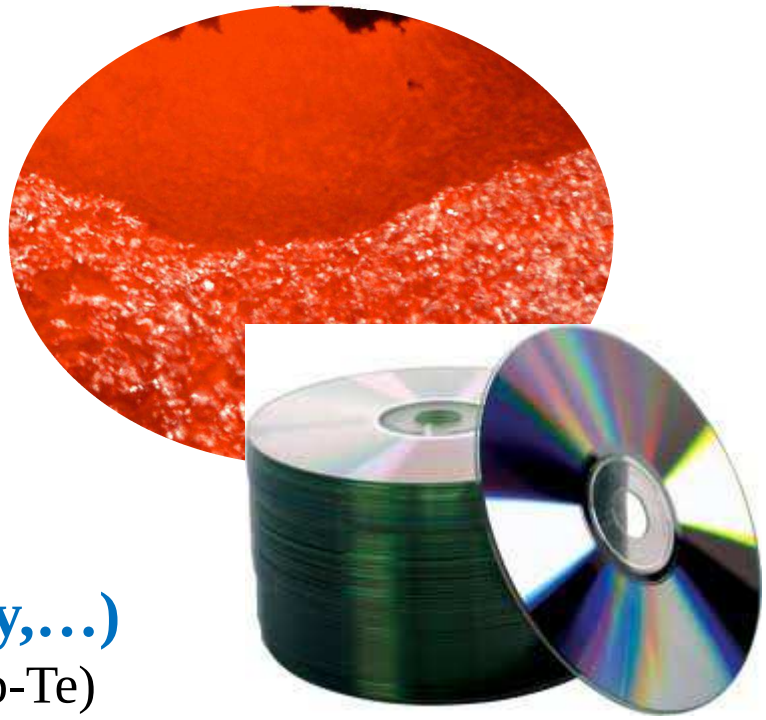


❑ (Thio)silicate glasses

- ➢ 10% Na_2O-15% CaO- 75%SiO_2 (window glass)
- ➢ Solid electrolytes/batteries (additives)
- ➢ Heat resistance (pyrex, nuclear waste glasses)
- ➢ Radiation resistance (Ba based)
- ➢ Bottles (aluminosilicates)

❑ Alumino-silicates

Magmas, natural glasses

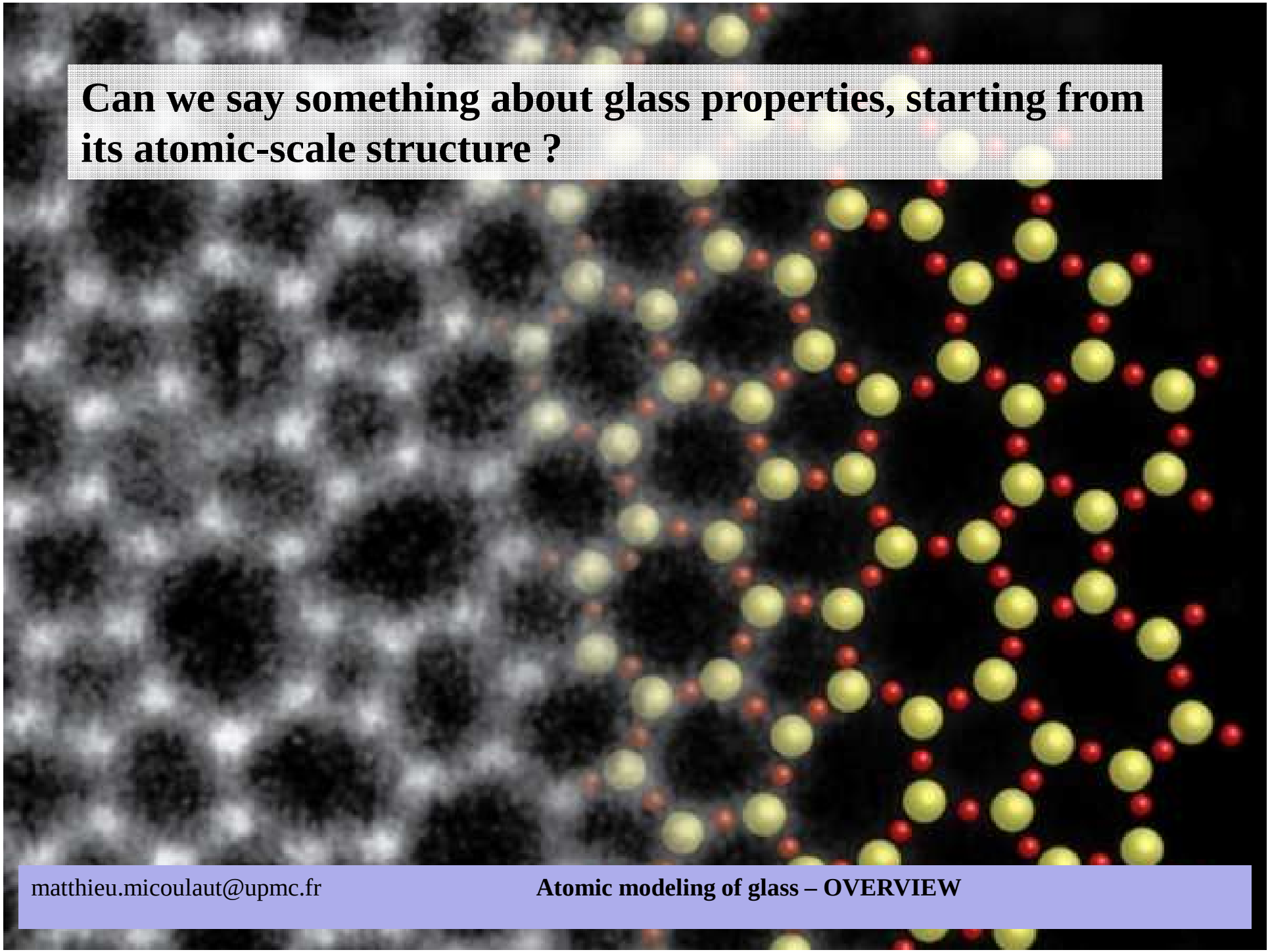


❑ Optical fibers

- pure SiO_2
- Tellurides, chalcohalides

❑ Data recording (DVD/Blue-ray,…)

- tellurides (Ge-Sb-Te, Ag-Ge-Sb-Te)


Can we say something about glass properties, starting from its atomic-scale structure ?

Outline of the course:

1. What is a glass, from liquids to glasses, basic models
2. Structural of glasses and experimental characterization
3. Simple bond models
4. Molecular Dynamics: Basics
5. Molecular Dynamics: Space correlation functions
6. Correlation functions and linear response

Outline of the course (con't):

7. Force fields and limitations

8. Practical MD and applications

9. Topological engineeering

10. Rigidity transitions and intermediate phases

11. Glassy dynamics

12. Ab initio simulations of glasses

13. Applications of ab initio simulations

Textbooks:

On glasses

- *Fundamentals of Inorganic Glasses*, Arun K. Varshneya
- *Physics of amorphous materials*, Stephen R. Elliott
- *Introduction to glass science and technology*, J.E. Shelby

On simulations

- *Glassy Materials and Disordered Solids*, W. Kob, K. Binder
- *Understanding Molecular Simulations*, D. Frenkel, B. Smit

Important link:

http://www.lptl.jussieu.fr/user/mmi/IMI_lecture

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