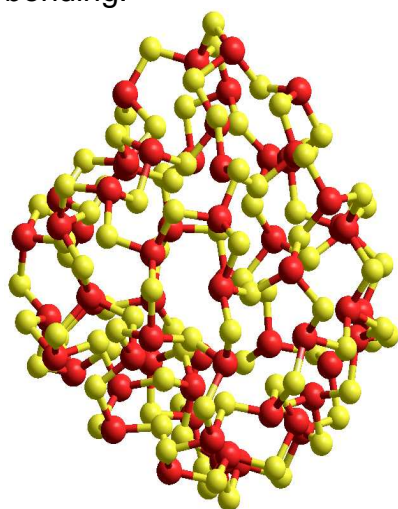


## Internship+PhD announcement

### Non volatile memories at the atomic scale: Structure, rigidity transitions and effect of composition.

**Context** : Amorphous telluride thin films are now present as starting material in many electronic devices and setups, and found huge applications in the phase change memory (DVD) industry. In order to design new material functionalities for (other) future applications such as improved infrared transmitting waveguides or stable phase change data storage, there is a demanding need to understand in more detail the underlying factors which control the glass-forming tendency of tellurides and the relationship between structure and functional properties. In contrast with light chalcogenides (selenium and sulphide) however, tellurides do not form easily bulk glasses due, in part, to a high crystallization tendency and a difference in chemical bonding.



**Proposed activity** : The present PhD project proposes to address such issues by combining molecular simulations and topological modeling of three important families of telluride glasses, with a special emphasis on compositional trends. The chosen alloys belong to the binary Ge-Te and the ternaries Ge-Sb-Te and Ge-Ga-Te systems since they are good candidates for phase change memory and infrared transmitting waveguides.

The projet will consist in an extensive study of compositional effects using ab initio Molecular Dynamics codes whose outputs (structure, dynamics, vibrational) will serve as inputs for topological modeling.

The theoretical effort will be achieved in parallel with an experimental one performed by collaborators. In a first stage, measurements of the liquid structure of selected compositions will be performed to validate the numerical schemes. During a second stage, guided by the theoretical predictions from topological models, it is planned to investigate experimentally compositional joins in the ternary phase diagrams which in turn will be compared with the outputs of the simulation.

Ultimately, it is expected to find (new) functionalities of amorphous tellurides, which could derive directly from the remarkable properties found in selected compositional regions, and which are well documented in selenide and sulphide glasses.

**Scientific environment** : The student will benefit from the expertise (MD simulations and statistical physics) of the LPTMC laboratory, located on the campus Jussieu in the historical center of Paris. The present announcement is part of a collaborative effort between french, american and german groups, combining experimental and theoretical contributions.

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