ABSTRACT PhD Project - Annalisa Pallini

Understanding Composition-Structure-Property Relationships to Design Ultra Strong AluminoSilicate Glasses.

Nowadays the development of ultrastrong glasses is a matter of huge interest because of the increasing demand for lightweight, ultrathin and durable glasses for applications such as cover and protective transparent materials for personal electronics, solar panels, sealants of electrochemical devices, screens, and windows for automobiles and aerospace vehicles, buildings etc.

Aluminosilicate glasses play a central role in all these applications since they possess high breakage resistance and chemical durability, high transparency, and low coefficient of thermal expansion.

Up to now, because of the gap of knowledge on composition-structure-properties relationships most of the commercial glasses have been designed by a conventional 'trial and error' approach. However, with an ever-increasing demand for new glasses with particular and tailored properties, it is becoming urgent to change the paradigm, from 'trial and error' to a more sustainable 'material by design' approach, whereby material functions and properties can be predicted from first principles. The project aims to develop a rigorous fundamental atomic level understanding of the relationships between composition structure and properties of these systems and to create some new very accurate, simple and efficient Force Fields.

Molecular Dynamics Simulations will be surely used to investigate A_2O–AEO–M_xO_y–Al_2O_3–SiO_2 (A: Li, Na; AE: Mg, Ca; M_xO_y: B_2O_3, and P_2O_5) glasses to understand the impact of (a) mixed network former effect, and (b) non-framework cation mixing on the glass properties (mechanical and coefficient of thermal expansion). Particular attention will be given to the understanding of processing conditions, such as densification through the application of hydrostatic pressure during glass production, and to Mechanical and Elastic properties.

The project will be carried out in tight collaboration with SCHOTT Glass; a leading international technology group in the areas of specialty glass, glass-ceramics and glass innovations which has manifested the interest in co-funding the scholarship and hosting

the PhD student for a period abroad of 6 months and providing experimental data necessary to validate our simulations.