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High-pressure and high-temperature effects in oxide glasses studied by complementary experimental and computational methods

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Glasses constitute a fascinating class of functional materials that lack translational symmetry and, therefore, exhibit isotropy in their various properties. It is noteworthy that one can synthesize amorphous analogues of various crystalline materials, finding applications in energy storage & conversion devices: batteries, fuel cells, supercapacitors, phosphors for light sources, etc. Furthermore, their random glass network allows for facile alteration of their properties, e.g. by applying high temperature (HT) and/or high pressure (HP). Preferably, such an optimized procedure leads to nanomaterials (glass-ceramics) with significantly improved properties, such as electrical conductivity, thermal conductivity, thermal stability, etc.

In this seminar, an overview of the synthesis and HPHT treatment of selected oxide glasses will be given, along with a description of the favorable properties of the obtained nanomaterials. Furthermore, it will be shown that computational simulations either help predict final results without a time-consuming "trial and error" approach or aid in understanding experimental results.