**Properties of P2O5 and phosphate glasses**

P2O5 represents an archetypal glass former, and when properly alloyed (phosphate glasses), one is able to develop a variety of specialty applications such as biocompatible materials for medical applications or lithium phosphate based fast ion conductors that make them useful as solid state electrolytes.

The final exam consists of a self-consisting report of ca. 10-12 pages (including figures and references) that each student will have to write and complete. The focus will be on the modeling of the structural properties of vitreous P2O5 and alkali phosphate glasses (Li2O-P2O5). The subject can be a mixture of multiple choice, topology and/or MD based studies, and/or case studies. The paper should compare the predictions of the simulations with the experimental findings, and discuss the cause of any differences observed.

As starting material, it is good to start with the following references:

1. *Review: the structure of simple phosphate glasses*, R.K. Brow, Journal of Non-Crystalline Solids 263-264, 1 (2000).
2. *Topology of alkali phosphate glass networks*, Anna I. Fu, J.C. Mauro, Journal of Non-Crystalline Solids 361, 57 (2013).
3. *The Molecular Dynamics Study of Lithium Ion Conduction in Phosphate Glasses and the Role of Non-Bridging Oxygen*, A. Karthikeyan, P. Vinatier, A. Levasseur, and K. J. Rao, J. Phys. Chem. B 103, 6185 (1999).
4. *Molecular dynamics simulation of the structure and properties of lithium phosphate glasses*, J.-J. Liang, R.T. Cygan, T.M. Alam, Journal of Non-Crystalline Solids 263-264, 167 (2000).
5. *Computer Simulation of Noncrystalline P2O5, an Ionic–Covalent Oxide*, D. K. Belashchenko\* and O. I. Ostrovskii, Inorg. Mater. 38, 48 (2002).
6. *Structural study of lithium phosphate glasses by X-ray RDF and computer simulations*, Ramesh K. Sistla, M. Seshasayee, Journal of Non-Crystalline Solids 349, 22 (2004).

Suggest 2 weeks for completion with due date Nov. 21, 2013, discretion of local adviser.