Abstract Submitted for the MAR12 Meeting of The American Physical Society

The effect of polar interactions on the dynamics in vitreous liquids ALEXANDER AGAPOV, YANGYANG WANG, PHILIP GRIFFIN, ALEXEI SOKOLOV, Department of Chemistry, University of Tennessee — It is known that in small molecule and polymeric systems the long-range process like diffusion and chain relaxation decouple from the local structural relaxation temperature dependence as system approaches its T_q . Recently, it was shown by Sokolov and Scweizer (Phys. Rev. Lett. 2009, 102, 248301) that these decoupling phenomena seem to have similar underlying mechanism irrespective whether system is a polymeric or a molecular liquid. The degree of decoupling for both polymers and small molecule systems show very similar trend with respect to the fragility of the material. More fragile systems show higher degree of decoupling. However, such behavior was shown only on the example of dynamics in weakly interacting van der Waals systems. On the example of three polymers and one room temperature ionic liquid (RTIL) it is demonstrated that the presence of polar interactions leads to rather steep temperature dependence of large length scale dynamic processes, like chain relaxation and self-diffusion. As a result, the degree of decoupling between large length scale and local dynamic processes in such polar materials is significantly lower than in weakly interacting liquids with comparable fragilities. The microscopic mechanism behind an unusual dynamic behavior seen in polar polymers and RTILs remains unclear. Nevertheless, knowledge of such structure-property relationship can significantly aid in the development of novel materials. Authors are thankful to NSF and (U.S.) DOE, Office of Basic Energy Sciences for the financial support.

> Alexander Agapov Department of Chemistry, University of Tennessee

Date submitted: 09 Nov 2011

Electronic form version 1.4