**Poster Presentation**

**MS060.P01**

*Exploring liquid-liquid' transitions in ZnSe at extreme conditions*

Sakura Pascarelli[1], Can Yildirim[2], Jean-Yves Raty[3], Innokenty Kantor[2], Raffaella Torchio[2], Angelika Dorothea Rosa[2], Gaston Garbarino[2], Gunnar Weck[4], Jean-Pierre Gaspard[3]

*[1]European Synchrotron Radiation Facility, Grenoble, France, [2]Esrf, Grenoble, France, [3]1SPIN-Université de Liège, Institut de Physique B5, 4000 Sart-Tilman, Belgium, [4]CEA, Paris, France*

E-mail: sakura@esrf.fr

Here, we report on the fingerprints of 4-fold to 6-fold transition in liquid ZnSe at extreme pressure and temperature conditions up to 42 GPa and more than 3000 K using X-ray absorption spectroscopy (XAS) combined with laser-heated diamond anvil cell techniques and complementary ab initio molecular dynamics simulations. Among pressure induced structural modifications, liquid–liquid' (L-L') transitions have attracted much interest both experimentally and theoretically due to their peculiarity. Unlike most L-L' transitions that only show slight modifications of the bond distances between atoms (i.e., P, Na, supercooled Si) [1, 2, 3], strong L-L' transitions have been theoretically predicted for a few II-VI semiconductor compounds such as ZnSe, CdSe and CdTe, given the following two conditions are satisfied: Firstly, the melting of the sp3 bonded phase (4-fold coordination) at ambient pressure results in a liquid structure that remains approximately 4-fold coordinated; and secondly, the presence of a semiconductor to metal phase transition under pressure [4, 5, 6, 7]. Our results show that solid and liquid ZnSe undergoes a series of structural modifications at various P, T values that satisfy the conditions above. The red shift in Zn K edge energy observed at around 7 GPa upon increasing temperature suggests a metallization event before melting to a possible 6-fold coordinated liquid structure. These findings are supported by our simulation results showing a pronounced difference in the first diffraction peak of the calculated structure factor at high pressures indicating a 4-fold to 6-fold coordination change in liquid ZnSe. Our results may provide additional insight for such transitions that may be observed for similar tetrahedrally coordinated II-VI systems.

[1] Raty, J.Y, Eric S., and Stanimir A. B. Nature 449.7161 (2007): 448-451.
[2] Katayama, Yoshinori, et al. Nature 403.6766 (2000) 170-173.
[3] Ganesh, P., and M. Widom. Physical review letters 102.7 (2009): 075701.
[4] T. Narushima et al., Joint 20th AIRAPT-43th EHPRG Proceedings (2005),
[5] T. Tsukatani, A. Chiba, K. Tsuji, Journal of Physics: Conference Series (2010): 215 012076.
[6] J.-P. Gaspard, J.-Y. Raty, R. Céolin and R. Bellissent, J. non Cryst. Solids, (1996): 205-207, 75-78
[7] Hattori, T., Kinoshita, T., Narushima, T., Tsuji, K., & Katayama, Y. (2006). Physical Review B, 73(5), 054203.

**Keywords:** Liquide-liquide phase transitions, laser-heated DAC, XAS