

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Mode coupling in liquid Zn. An ab-initio molecular dynamics study.¹ BEATRIZ GONZALEZ DEL RIO, LUIS E. GONZALEZ, DAVID J. GONZALEZ, Universidad de Valladolid — The static and dynamic properties of liquid Zn have been studied using an ab initio molecular dynamics method. Results are reported for the thermodynamic states at 723 K for which inelastic neutron scattering data are available [1]. The calculated static structure shows very good agreement with experimental measurements, including an asymmetric second peak. The dynamic structure reveals the existence of a second propagating mode in both the longitudinal and transverse current correlation functions. We explain this anomaly, previously observed in other liquid metals under high pressure [2], using Sjgren and Sjlander mode coupling theory (MCT) [3]. The MCT provides a satisfactory description of the results although, it lacks accuracy in some wavevector regions. Nevertheless, it provides a first step in the understanding of an interesting phenomenon that is starting to be observed in liquid metals and that, up to now, was thought to only appear at high pressures. [1] M. Zanatta et al, Phys. Rev. Lett. 114, 187801 (2015) [2] T. Bryk et al, J. Chem. Phys. 143, 104502 (2015); M. Marqus et al, J. Phys. Condens. Matter 28, 075101 (2016) [3] L. Sjgren, Phys. Rev. A 22, 2883 (1980)

¹We acknowledge MEC (FIS2014-59279-P) and Universidad de Valladolid.

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Date submitted: 08 Nov 2016

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