

Abstract Submitted  
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**Static structure, microscopic dynamics and electronic properties of liquid titanium near melting. An ab-initio study<sup>1</sup>** DAVID J. GONZALEZ, BEATRIZ GONZALEZ DEL RIO, LUIS E GONZALEZ, Dept Fisica Teorica, Atomica y Optica, Facultad de Ciencias — We present an ab-initio molecular dynamics study of several structural, dynamic and electronic properties of liquid titanium near melting. The obtained structural results are compared with the available experimental data, most notably the static structure factor for which discordant experimental data have been reported [1]. Several dynamical properties have been calculated, such as the velocity autocorrelation function, intermediate scattering functions and dynamic structure factors along with some transport coefficients. The dynamic structure factors show side peaks indicative of collective density excitations and the associated dispersion relation curve has been compared with experiment. The relaxation mechanisms for the density excitations have been analyzed in terms of a model with two decay channels. [1] Y Waseda, The Structure of Non-Crystalline Materials, (New York: McGraw-Hill, 1980); K F Kelton et al, Phys Rev. Lett. 90, 195504 (2003); D Holland-Moritz et al, Mater. Sci. Eng. A, 449-451, 42 (2007)

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David J. Gonzalez  
Dept Fisica Teorica, Atomica y Optica, Facultad de Ciencias

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