Abstract Submitted
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Ab-initio study of the structure and dynamics of bulk liquid Cadmium and its liquid-vapour interface[1] DAVID J. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN, LAZARO CALDERIN, Materials Research Institute and Research Computing and Cyberinfrastructure, The Pennsylvania State University, Pennsylvania 16802, USA, LUIS E. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN — Several static and dynamic properties of bulk liquid cadmium at a thermodynamic state near its triple point have been calculated by *ab-initio* molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data. The dynamical structure reveals collective density excitations with an associated dispersion relation which points to a small positive dispersion. Results are also reported for several transport coefficients. Additional simulations have also been performed in order to study the structure of the free liquid surface. The ionic density profile shows an oscillatory behavior with two different wavelengths as the spacing between the outer and first inner layer is different from that between the other inner layers. The calculated reflectivity shows a marked maximum whose origin is related to the surface layering along with a shoulder located at a much smaller wave-vector transfer.

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