Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Orbital-free ab initio molecular dynamics study of the free liquid surface of Cd. BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, Fisica Teorica, Atomica y Optica, Universidad de Valladolid — We report results of an orbital-free *ab initio* molecular dynamics (OF-AIMD) study of the free liquid surface of Cd at 800 K. A key ingredient in the OF-AIMD method is the local ionic pseudopotential describing the ions-valence electrons interaction. We have developed a force-matching method [1] to derive a local ionic pseudopotential suitable to account for a rapidly varying density system, such as a free liquid surface. Results are reported for several structural properties. The calculated reflectivity shows a marked maximum whose origin is related to the surface layering, along with a shoulder located at a much smaller wavevector transfer. [1] B. G. del Rio and L. E. Gonzalez, J. Phys.: Condens. Matter **26**, 465102 (2014)

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Date submitted: 04 Nov 2015 Electronic form version 1.4