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Orbital-free ab initio molecular dynamics study of the free liquid surface of Sn. From pseudopotential generation to structural and dynamic properties[1] BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, Universidad de Valladolid — We report results of an orbital-free ab initio molecular dynamics (OF-AIMD) study of the free liquid surface of Sn at 1000 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 in a free liquid surface. We obtain very good results for several structural properties. We have also studied the evolution of some dynamical properties when going from the central region (where the system behaves like the bulk liquid) towards the free liquid surface.

[1] B.G. del Rio and L.E. Gonzalez, J.Phys.:Condens. Matter 26, 465102 (2014)

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