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Orbital-free ab initio molecular dynamics study of the dynamics of the free liquid surface of In.[1] BEATRIZ GONZALEZ DEL RIO, LUIS E. GONZALEZ, DAVID J. GONZALEZ, Universidad de Valladolid — We report results of an orbital-free ab initio molecular dynamics (OF-AIMD) study of the free liquid surface of In at 550 K. A key ingredient in the OF-AIMD method is the local pseudopotential describing the ions-valence electrons interaction. We have used the previously developed 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. We obtain good results for structural properties, such as the reflectivity. Moreover, we have been able to study ab initio the evolution in some dynamical properties as we move from the central region where the system behaves like the bulk liquid, to the free liquid surface and compare them to experimental results [2].
[1] B.G. del Rio and L.E. Gonzalez, J. Phys.: Condens. Matter 26, 465102 (2014)
[2] B. Wehinger, M. Krisch, and H. Reichert, New Journal of Physics 13, 023021 (2011)

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