Abstract Submitted
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***Ab initio* molecular dynamics simulations of the static, dynamic and electronic properties of liquid Bi**[1] JAIME SOUTO, M.M.G. ALEMANY, L.J. GALLEGO, Universidad de Santiago de Compostela, Spain, L.E. GONZALEZ, D.J. GONZALEZ, Universidad de Valladolid, Spain — We perform a comprehensive study of the static, dynamic and electronic properties of liquid Bi near melting by means of 124-atom *ab initio* molecular dynamics simulations based on PARSEC, a real-space implementation of pseudopotentials constructed within the density-functional theory. The predicted results are in good agreement with available experimental data, thus confirming the adequacy of this technique to achieve a reliable description of a non-simple liquid metal such as liquid Bi, whose static structure has reminiscences of the rhombohedral structure of the crystal. Our results for the intermediate scattering function, density of states and electrical conductivity also show markedly differences to those of simple liquid metals.

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