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***Ab initio* molecular dynamics simulations of the static, dynamic and electronic properties of liquid lead**[1] L.J. GALLEGO, MANUEL ALEMANY, R.C. LONGO, Universidad de Santiago de Compostela, Spain, D.J. GONZALEZ, L.E. GONZALEZ, Universidad de Valladolid, Spain, MURILO L. TIAGO, Oak Ridge National Laboratory, JAMES R. CHELIKOWSKY, University of Texas at Austin — We present results for a comprehensive study of the static, dynamic and electronic properties of liquid Pb near melting by means of 216-particle *ab initio* molecular dynamics simulations based on a real-space implementation of pseudopotentials constructed within density-functional theory. The predicted results and available experimental data are in very good agreement, which confirms the adequacy of this technique to achieve a reliable description of the behavior of liquid metals, including their dynamic properties. Although some of the computed properties of liquid Pb are similar to those of simple liquid metals, others differ markedly. Our results show that an appropriate description of liquid Pb requires the inclusion of relativistic effects in the determination of the pseudopotentials of Pb.

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