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Ab initio molecular dynamics simulations of the static, dynamic and electronic properties of the liquid Bi-Pb alloy[1] J. 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 an ab initio molecular dynamics study of the static, dynamic and electronic properties of the liquid Bi-Pb alloy at three concentrations, including the eutectic one. This alloy is of particular technological interest for its possible use as coolant in fast reactors. Our predictions are in good agreement with the available experimental data. In particular, the computed total static structure factors reproduce accurately the neutron diffraction results, and the predicted adiabatic sound velocity and shear viscosity compare well with the experimental values. The partial dynamic structure factors exhibit clear side peaks indicative of propagating density fluctuations, and the longitudinal and transverse dispersion relations show several branches.The electronic density of states show that the liquid Bi-Pb alloy is a good metal, but with strong deviations from the free-electron parabolic curve.

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