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Melting behaviour of high pressure Na. An ab initio study DAVID J. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid, LUIS E. GONZALEZ, Dpt Fisica Teorica, Universidad de Valladolid, Valladolid — The melting curve of sodium for a pressure range up to 120 GPa has been evaluated by the orbital free ab initio molecular dynamics method. This method uses the electronic density as the basic variable and scales almost linearly with system size which allows to perform simulations with a large number of particles and for long simulation times. For various pressures and temperatures we have calculated some static properties (pair distribution functions, static structure factors and short-range order parameters), dynamic properties (mean square displacement, velocity autocorrelation functions and dynamic structure factors) and transport coefficients (self-diffusion, adiabatic sound velocities and shear viscosities). The calculated melting curve reproduces the main qualitative features found in the experiment.

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