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An ab initio study of the structure and dynamics of bulk liquid Ag and its liquid-vapor interface. BEATRIZ GONZALEZ DEL RIO, LUIS ENRIQUE GONZALEZ TESEDO, DAVID JOSE GONZALEZ FERNANDEZ, Fisica Teorica, Atomica y Optica, Universidad de Valladolid — Several static and dynamic properties of bulk liquid Ag at a thermodynamic state near its triple point have been calculated by means of *ab initio* molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data. The dynamical structure reveals collective density excitations with an associated dispersion relation which points to a small positive dispersion. Results are also reported at a slightly higher temperature in order to study the structure of the free liquid surface. The ionic density profile shows an oscillatory behaviour with two different wavelenghts, as the spacing between the outer and first inner layer is different from that between the other inner layers.

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