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Ab-initio study of the free liquid Hg surface LAZARO CALDERIN, Research Computing and Cyberinfrastructure, Penn State, University Park 16802, PA, USA, LUIS E. GONZALEZ, DAVID GONZALEZ, University of Valladolid, Valladolid, Spain — The free surface of liquid Hg at two temperatures (T=300 and 450 K) has been studied by using first principles molecular dynamics simulations. The calculated longitudinal ionic density profile shows an oscillatory shape extending several atomic diameters into the bulk and its wavelength is in good agreement with experiment. The associated self-consistent valence electronic density profile shows much weaker oscillations which are somewhat out of phase with the ionic ones. The calculated X-ray reflectivity shows a marked maximum at a wavevector transfer of $q_z \approx 2.2$ Å^{-1} whose origin is related to the surface layering. Moreover, it shows a good agreement with the experimental reflectivity data.

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