

Theoretical and experimental study of the dynamical electronic response of Ag

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Abstract

In this paper we present theoretical and experimental results for the linear electronic response of Ag. The calculations are performed within time-dependent density-functional theory. They are based on a pseudopotential scheme with and without the inclusion of semicore states and a plane-wave expansion of the wave functions. The influence of the semicore states is shown and discussed. The results for the ground-state calculation are furthermore compared to those of all-electron calculations. The theoretical results are then compared to EELS spectra obtained using a transmission electron microscope. Although we achieve good agreement in many aspects it is shown that even for such a supposedly simple material as crystalline Ag the results cannot be fully understood.