Non-local study of exchange-correlation holes in model metal surfaces

Dominik B. Jochym and Stewart J. Clark

Department of Physics, Durham University
Durham, UK

The popularity of local and semi-local density functionals has seen them applied to many types of system, including those that are expected to rely heavily on non-local effects. Accurate simulations of surface systems, in particular, are important to understand processes such as catalysis. The weighted density approximation[1,2] (WDA) is a fully non-local density functional, which is implemented in a developmental version of CASTEP[3]. Here we apply the WDA to a jellium surface and a Cu(100) surface, with aim to observe the behaviour of the exchange-correlation hole. We show that there are significant non-local effects, meriting further study of surfaces using functionals such as the WDA.

[1] J.A. Alonso and L.A. Girifalco, Solid State Commun. **24**, 135 (1977).

[2] O. Gunnarsson, M. Jonson, and B.I. Lundqvist, Solid State Commun. **24**, 765 (1977).

[3] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, and M. C. Payne, J. Phys.: Condens. Matter **14**, 2717 (2002).