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GW quasiparticle energy calculations for surfaces: the influence of polarization effects in a repeated-slab approach PHILIPP EGGERT, CHRISTOPH FREYSOLDT, PATRICK RINKE, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, ARNO SCHINDLMAYR, Forschungszentrum Jülich, Germany — The combination of density functional theory (DFT) and many-body perturbation theory in the GW approximation has become an important tool for *ab-initio* band structure calculations typically in good agreement with experiment. In order to treat surfaces one often employs a repeated slab geometry for computational convenience. However, electric multipole moments may occur in the slabs which then lead to a slowly decaying electrostatic interaction. If present, static dipoles must be corrected for in DFT [1]. In GW however, dynamic dipoles are always created. We present calculations for the hydrogen-saturated silicon (001) slabs and show that slabs smaller than 10 layers are not converged fully with 10-20 Å vacuum thickness. The effect of the dynamic dipoles is slowly decreasing with slab thickness, in accordance with an extension of a simple electrostatic model, that includes these polarization effects [2]. Therefore it is essential to monitor the convergence carefully and if necessary to extrapolate to infinite separation.
[1] J. Neugebauer, M. Scheffler, Phys. Rev. B **46**, 16067 (1992)
[2] C. Delerue, G. Allan and M. Lannoo, Phys. Rev. Lett. **90**, 076803 (2003)

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