Homework 5: Computational Design of Materials

Due: January 15, 2013

Work function on a hydrogen-terminated and chlorine-terminated diamond (100) surface.

Negative-electron-affinity (NEA) surfaces are semiconductor surfaces that have a work function such that the vacuum level lies below the conduction-band edge. Electrons that are present in the conduction band can therefore readily escape the surface. The NEA surfaces are utilized in a number of important applications, such as photocathodes, secondary electron emitters, and cold-cathode emitters. In general, wide-band-gap semiconductors are particularly suitable candidates for NEA emitters, since the conduction-band minimum is likely to be close to the vacuum level. Diamond, with a 5.5-eV band gap can be grown as high-quality films, both homoepitaxially on (100) substrates and highly oriented textured films on (100) silicon surfaces.

Calculate the work function on a hydrogen-terminated diamond (100) surface. Discuss the physics underlying your simulation result. Repeat the simulation on a chlorine-terminated diamond (100). What is the difference in work functions on the two surfaces? Explain the underlying physics that results in the difference.