Semi-infinite solid approach to calculations of surface properties

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A method for carrying out electronic density functional theory calculations of surface properties using a semi-infinite solid model and a fixed chemical potential of electrons is presented along with various applications to metal and semiconductor surfaces. A Green function approach [1] is used to simulate a system consisting of two regions: (A) the bulk solid represented by a minimal unit cell and subject to periodic boundary conditions in three dimensions, and (B) a surface region represented by a few atomic layers subject to periodic boundary conditions in two dimensions with a free surface on one side but matched to region (A) on the other side. Not only is this a more accurate description of a solid surface but the computational effort is also an order of magnitude smaller than with the commonly used slab model. The semi-infinite solid approach has been implemented in the ATK software using atomic basis sets. Results of calculations demonstrate fast and system atic convergence of, for example, work function and band gap with the number of layers in region (B), while results of slab calculations show erratic convergence or even lack of convergence with the number of layers in a slab. This new methodology opens up new possibilities for simulating the properties of thin films and nanostructures on surfaces where the coupling to the substrate is properly taken into account.

[1] M. Brandbyge, J-L. Mozos, P. Ordejon, J. Taylor, and K. Stokbro, *Phys. Rev. B* **65**, 165401 (2002).