DFT simulations of surfaces, interfaces and multilayers

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I'll give a brief introduction into the underlying concepts of solid state modeling using periodic boundary conditions and then describe the strong and weak points of Density Functional Theory (DFT), and some routes to overcome its limitations. Then I'll discuss various spectroscopies which can be simulated using such quantum mechanical calculations and in particular using our WIEN2k code (www.wien2k.at) like XPS, XANES and EELS or UV/Vis spectroscopies using some specific examples. Finally I'll describe the reconstruction of a new surface model of the Fe_3O_4 (001) surface and a $SrTiO_3/LaVO_3$ multilayer system, which we propose as a possible photovoltaic material.