Extended Systems in Electrostatic Fields

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The basic principles behind a theoretical method for treating infinite, periodic systems exposed to an external electrostatic field are outlined. The approach, based on the vector-potential description of the external field, leads to single-particle Hartree-Fock or Kohn-Sham equations that differ from the field-free counterparts in several aspects. In particular, solving them is only possible through a careful so-called smoothing procedure. In that case it is possible to derive a numerically stable and efficient approach. Results of model studies as well as of the first *ab initio* calculations, in both cases for quasi-one-dimensional systems, are reported in order to illustrate the approach. Although the approach is based on the treatment of infinite, periodic systems, it is demonstrated that effects of the terminations are included. Finally, extensions to two- and three-dimensional systems are discussed, where surfaces and shapes turn out to have surprising effects.

Details of the work are presented in the following references:

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