

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Infinite, periodic systems in external fields – an efficient, theoretical method MICHAEL SPRINGBORG, University of Saarland, Germany — The response of periodic systems to external electric fields is a challenging theoretical problem. We show how the vector potential approach yields a numerically efficient treatment of the combined electronic and nuclear response to a finite static field. Our method is based on a self-consistent reformulation of the charge flow term in the single particle Hamiltonian. Careful numerical implementation yields a treatment whose computational needs are only marginally larger than those of a conventional field-free calculation. To prove the method we have performed model calculations for a quasi-one-dimensional (polymeric) system. The model contains all essential elements of an ab initio Kohn-Sham or Hartree-Fock Hamiltonian but allows for extensive testing.

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Date submitted: 15 Nov 2006

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