Implementation of a vector potential method in an *ab initio* Hartree-Fock code

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For extended systems exposed to an external, electrostatic field, the presence of the field leads to an extra term ($\vec{E}$. $\vec{P}$) to the Hamiltonian, where $\vec{E}$ is the field vector and $\vec{P}$ is the polarization of the system of interest. In order to find out how a polymer chain responds to an external electric perturbation, a field with a charge and a current term for the polarization is added to an *ab initio* Hartree-Fock Hamiltonian. The polarization expression is taken from an efficient vector potential approach (VPA) for calculating electronic and nuclear responses of infinite periodic systems to finite electric fields and is implemented in the *ab initio* LCAO-SCF algorithm, which computes band structure of regular or helical polymers, taking into account the one-dimensional translational symmetry.

Literature:

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