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Going beyond Kohn and Sham (KS): determining accurate ground and first excited states LUIZ FERREIRA, Universidade de Sao Paulo, MARCELO MARQUES, LARA TELES, RONALDO PELA, Instituto Tecnologico de Aeronautica — The Total energy in KS is written as

$$E = \frac{1}{2}\sum \int \nabla\psi^* \cdot \nabla\psi + \frac{1}{2}\int \frac{\sum \psi^*\psi(r) \sum \psi^*\psi(r')}{(r-r')} + \int \sum \psi^*\psi V_{nuclei} + Exc$$

The KS procedure continues by minimizing the energy with respect the wavefunctions ψ. The equation for the wave functions is similar to the one-particle Schroedinger equation. In our talk we will present results obtained in the following way: we add an external potential V_{add} to the nuclei potential V_{nuclei} and, after the calculation is completed, we subtract what we added, namely. $-\int \sum \psi^*\psi V_{add}$. The result is a calculation according to the Eq. above but with wavefunctions not satisfying the KS equations. If the exchange-correlation term were reliable one would expect that the calculated energy would be larger than the KS energy. The added potential V_{add} is what is being used in the *LDA-1/2* method and is dependent on a cut-off parameter C. Making the extremization of the total energy with respect to C we obtain (1) a point of maximum, which frequently will be shown to be the first excited state, (2) a minimum, with an energy lower than the KS ($C = 0$) ground state and with improved lattice parameter.

Luiz Ferreira
Universidade de Sao Paulo

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