Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**A systematically improvable second-principles method including electron and lattice degrees of freedom** PABLO GARCIA-FERNANDEZ, Departamento CITIMAC, Universidad de Cantabria, Avenida de los Castros s/n, 39005 Santander, Spain, JACEK WOJDEŁ, JORGE ÍÑIGUEZ, Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, E-08193 Bellaterra, Spain, JAVIER JUNQUERA, Departamento CITIMAC, Universidad de Cantabria, Avenida de los Castros s/n, 39005 Santander, Spain — One of the most difficult tasks when trying to expand Density Functional Theory (DFT) calculations to large systems is the scaling of computational time with the number of electrons in the simulation box. However, not all electrons play a relevant role in the determination of the physical magnitude under scrutiny. In this work we present a systematic approximation to DFT based on a rigorous separation of these active electrons and holes from those of a reference state. Using a similar expansion to that found in Tight-binding DFT methods we obtain a large term containing the energy of the reference system, and a second, much smaller one, associated to the active part of the electron density. We associate the energy of the reference system to the lattice degrees of freedom and use a well-tested model Hamiltonian to represent them, on the other hand, the active electrons are described using a small but accurate Wannier function basis-set. Combined with an efficient Lanczos-based diagonalization, our method provides a systematically improvable scheme to simulate systems including tens of thousands of atoms under experimental conditions. We provide several examples of its application in the field of transition-metal oxides.

Pablo Garcia-Fernandez
Departamento CITIMAC, Universidad de Cantabria,
Avenida de los Castros s/n, 39005 Santander, Spain

Date submitted: 11 Nov 2014 Electronic form version 1.4