Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Relaxation of atomic orbitals in a plane-wave basis set JOSE LUIS MARTINS, Departamento de Física, Instituto Superior Técnico, Universidade de Lisboa, and INESC-MN, Lisboa, Portugal, CARLOS L. REIS, INESC-MN, Lisboa, Portugal — We investigate a first-principles calculations scheme that uses a small or even minimal atomic orbital basis-set which is expanded in plane-waves and is subsequently augmented by a simple relaxation procedure in that same plane-wave basis set. Our results show good agreement between the standard pseudopotential plane-wave method and the novel hybrid methodology. The proposed method is simple to implement in existing plane-wave computer programs and leads to substantial gains in computation speed while maintaining reasonable accuracy. We show results for some test cases, including local-density band-structures of silicon and graphite and radial distribution functions of liquid silicon.

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Date submitted: 12 Nov 2013 Electronic form version 1.4