Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Consistent treatment of charged systems within periodic boundary conditions: The Projector Augmented-Wave and pseudopotential methods revisited JEAN-PAUL CROCOMBETTE, FABIEN BRUNEVAL, CEA, DEN, Service de Recherches de Metallurgie Physique, F-91191 Gif-sur-Yvette, France, XAVIER GONZE, European Theoretical Spectroscopy Facility, Institute of Condensed Matter and Nanosciences, Universite catholique de Louvain, Chemin des Etoiles 8, BORIS DORADO, MARC TORRENT, FRANCOIS JOLLET, CEA, DAM, DIF, F-91297 Arpajon, France — The *ab initio* calculation of charged defect properties in solids is not straightforward because of the delicate interplay between the long-range Coulomb interaction and the periodic boundary conditions. We derive the Projector Augmented-Wave (PAW) energy and hamiltonian with a special care on the potentials from Coulomb interaction. By explicitly treating the background compensation charge, we find a new term in the total energy of charged cells and in the potential. We show that this background term is needed to accurately reproduce all-electron calculations of the formation energy of a charged defect. In particular, the previous PAW expressions were spuriously sensitive to the pseudization conditions and this artifact is removed by the background term. This PAW derivation also provides insights into the norm-conserving pseudopotential framework. We propose then an alternative definition for the total energy of charged cells and for the potential within this framework.

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Date submitted: 12 Nov 2013 Electronic form version 1.4