Abstract Submitted
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Unique assignment of energy to atoms in a solid MIN YU, DALLAS R. TRINKLE, RICHARD M. MARTIN, University of Illinois, Urbana-Champaign — We propose a way to decompose the total energy in a material into the contribution associated with each of the atoms, using the first-principles energy density formalism [1]. Although the energy density function is non-unique up to a gauge transformation, it has been used to calculate surface energies by integrals over cells chosen by symmetry [1] or over Voronoi polyhedra [2]. Bader charge analysis [3] partitions space into regions with a unique intergrated energy for any system with no requirements of symmetry. We implement the energy density method in the Vienna ab initio simulation package (VASP [4]) for both US-PP and PAW. We calculate energies for the Si (111), GaAs (110) nonpolar and (111) polar surfaces; vacancies and interstitials in Si and Al; and O in Ti. [1] N. Chetty and Richard M. Martin, Phys. Rev. B 45, 6074 (1992). [2] K. Rapcewicz, et al., Phys. Rev. B 57, 7281-7291(1998). [3] R. F. W. Bader, Atoms in Molecules: A Quantum Theory (1990). [4] G. Kresse and D. Joubert, Phys. Rev. B 59, 1758 (1999).

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