Abstract Submitted
for the TSF16 Meeting of
The American Physical Society

Recent Developments in Computing the Properties of Atoms in Materials[1] NIDIA GABALDON LIMAS, TAOYI CHEN, THOMAS MANZ, New Mexico State University — Recent advances in computing power are making it ever more practical to use quantum chemistry methods to study complex materials. A key challenge is to extract meaningful insights from the results of these computations. Although net atomic charges (NACs), bond orders, and magnetic moments are widespread chemical concepts, their computation requires specialized methods. The Density Derived Electrostatic and Chemical (DDEC) method optimizes atomistic descriptors to accurately reproduce both the chemical states of atoms in materials and the force fields surrounding the material. This makes them ideally suited both for studying the chemical properties of materials and for constructing force-fields used in classical molecular dynamics or Monte Carlo simulations. The latest generation of this method, called DDEC6, offers substantial improvements in accuracy and computational cost compared to prior generations. The DDEC6 method assigns NACs, atomic spin moments, effective bond orders, atomic multipole moments, polarizabilities, and dispersion coefficients using only the total electron and spin distributions of the material as inputs. To assess the accuracy of this approach, comparisons of computed to experimental results will be presented for a broad range of periodic and non-periodic materials.

[1]Support for this work was provide by NSF grant DMR-1555376.

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Date submitted: 29 Sep 2016 Electronic form version 1.4