Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

A generalization of the charge equilibration method RAZVAN A. NISTOR, JELIAZKO G. POLIHRONOV, MARTIN H. MUSER, NICK J. MOSEY, Department of Applied Mathematics, University of Western Ontario — Charge-equilibration (C-Eq) methods are an efficient means of calculating the effective partial charges of the atoms in molecules. The aim of obtaining the partial charges is to reconstruct the electrostatic field of a molecule, which then may be used as an accurate replacement to *ab initio* interatomic potentials. However, the inability of the C-Eq method to consistently predict the correct charges for a wide range of molecular geometries has limited its potential use in molecular simulations. A generalization to a split charge (split-Q) formalism, where the semi-empirical fit parameters are defined not in terms of atom-type, but in terms of bond-type, greatly improves the quality, and more importantly, the transferability of the fits. The flexible formalism of the split-Q approach allows for a number of generalizations over traditional C-Eq methods at the cost of additional fit parameters in the model. However, the split-Q approach can reproduce the charges on a variety of different molecules containing H, C, O, and Si, up to three times more accurately than previous methods when comparing to *ab initio* calculations.

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Date submitted: 19 Nov 2005 Electronic form version 1.4