Abstract Submitted
for the TSS15 Meeting of
The American Physical Society

A Novel Gaussian-*Sinc* mixed Basis Set for Electronic Structure Calculations JONATHAN JERKE, YOUNG LEE, C.J. TYMCZAK, Texas Southern Univ — A Gaussian-Sinc mixed basis set for the computation of the electronic structure atoms and molecules is presented. Excellent bases functions are known "core" and "valence" separately, such as Gaussians for the "core" wave and Plane-waves for "valance" wave functions, but as yet no is known that can accurately deal with both regimes in a single basis. A Sinc mixed basis can do both. This method resolves several issues such : i) the Sincs basis spans the same space as the plane-waves basis, yet are local enough to define all interaction elements including Exchange; ii) Gaussians span the spherically symmetric core states and can be mixed with Sinc functions in a computationally efficient methodology; iii) together, mixed basis set is a flexible, computationally efficient and a highly method for solving atomic and molecular problems. This methodology has implemented within the Hartree-Fock level of theory within ultra-strong fields. To demonstrate the utility of this new method, we calculated ground state Hartree-Fock energies to five digits accuracy in ultra strong fields for Helium to Neon, Molecular Hydrogen, Water, Carbon dioxide Benzene.

Jonathan Jerke
Texas Southern Univ

Date submitted: 26 Jan 2015 Electronic form version 1.4