

Abstract Submitted  
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**A Novel Gaussian-Sinc mixed Basis Set for Electronic Structure calculations**<sup>1</sup> JONATHAN JERKE, YOUNG LEE, C.J. TYMCZAK, Texas Southern University — A Gaussian-Sinc mixed basis set for the computation of the electronic structure of atoms and molecules is presented. Excellent bases functions are known for “core” and “valence” separately, such as Gaussians for the “core” wave functions and Plane-waves for “valance” wave functions, but as yet no method is known that can accurately deal with both regimes in a single basis. A Gaussian-Sinc mixed basis can do both. This method resolves several issues such as: i) the Sincs basis spans the same space as the plane-waves basis, yet are semi-local enough to define all interaction elements including Exchange; ii) the Gaussians span the spherically symmetric core states and can be mixed with the Sinc functions in a computationally efficient methodology; iii) together, this mixed basis set is a flexible, computationally efficient and a highly accurate method for solving atomic and molecular problems. This methodology has been implemented within the Hartree-Fock level of theory within ultra-strong magnetic fields. To demonstrate the utility of this new method, we calculated the ground state Hartree-Fock energies to five digits accuracy in ultra strong magnetic fields for Helium to Neon, Molecular Hydrogen, Water, Carbon dioxide and Benzene.

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