

Abstract Submitted
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**Hydrogen Dissociation in Generalized Hartree-Fock Theory:
Breaking the diatomic bond**¹ JONATHAN JERKE, Texas Southern University, SAMINA MASOOD, University of Houston Clear Lake, CJ TYMCZAK, Texas Southern University — Generalized Hartree Fock theory predicts molecular Hydrogen dissociation without correlation. A variational Gaussian-Sinc linear superposition is the basis of 50 calculations with 3-4 significant digits of quality. The spin singlet covalent bond spontaneously breaks into a pair of uncorrelated doublets at atomic separation of 1.22 Angstroms. Quantum spin numbers and energetic comparison with Configuration Interaction theory—correlation—point to a first order phase transition in the molecular Hydrogen bond without correlation.

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