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**Gutzwiller density functional theory for solid hydrogen calculations** JUN LIU, YONGXIN YAO, CHEN LIU, Ames Laboratory, DOE & Iowa State University, WENCAI LU, Qingdao University, PRC, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory, DOE & Iowa State University — We have recently proposed a Gutzwiller density functional theory (G-DFT) by innovatively replacing the noninteracting trial wavefunction in Kohn-Sham DFT with the Gutzwiller projected trial wavefunction to explicitly account for correlation effects, which renders a renormalized correlation matrix in the calculation as the key ingredient in our theory. Our approach does not require adjustable Coulomb interaction parameters, nor need of double counting terms present in LDA+U and LDA+DMFT. Our method has been demonstrated to work well in hydrogen and nitrogen molecule systems. In the presentation we will show its performance on the Hydrogen solid by specifically work out the total energy curves for different phases discussed in the literature, and compare them against the benchmark Quantum Monte Carlo (QMC) calculations.

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