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QMC Benchmarks of Density Functionals for High-Pressure Hydrogen Applications RAYMOND CLAY, Univ of Illinois - Urbana, JEREMY MCMINIS, Lawrence Livermore National Laboratory, JEFFREY MCMAHON, Univ of Illinois - Urbana, CARLO PIERLEONI, University of L'Aquila, DAVID CEPERLEY, Univ of Illinois - Urbana, MIGUEL MORALES, Lawrence Livermore National Laboratory — It has recently been shown in high-pressure hydrogen that the predicted locations of the liquid-liquid phase transition and the solid insulator-to-metal transition are very sensitive to the choice of density functional employed. We use Quantum Monte Carlo to benchmark some of the most commonly used DFT functionals for dense hydrogen in these two regions of the phase diagram. We find that in both of these phases, van der Waals and hybrid functionals noticeably outperform LDA and PBE functionals, and recommend the use of the vdW-DF [M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004)] functional for structural relaxation and molecular dynamics. We look at the impact of the functional on enthalpies, bond lengths, and the location of the liquid-liquid phase transition.

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