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Quasi-particle corrections to the LSDA+U electronic structure of solid bcc hydrogen EMMANOUIL KIOUPAKIS[1], PEIHONG ZHANG, STEVEN G. LOUIE, University of California, Berkeley and Lawrence Berkeley National Laboratory — Quasi-particle calculations within the GW approximation usually start with the LDA electronic structure as mean field solution, which works well for moderately correlated materials. For strongly correlated systems, such as the transition metal oxides, LSDA can give qualitatively wrong ground states, making any further improvement difficult. By starting with the LSDA+U mean field results in the GW approximation calculation of the electron self-energy, we expect to have a better understanding of the quasi-particle properties in these systems. We employ this approach in the study of solid hydrogen, a model system for which previous results exist in the literature. This will test the applicability of the technique to more realistic systems. This work was supported by National Science Foundation Grant No. DMR04-39768 and by the Director, Office of Science, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Computational resources have been provided by NSF at the National Partnership for Advanced Computational Infrastructure (NPACI) and DOE at the National Energy Research Scientific Computing Center (NERSC)

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