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Noncovalent hydrogen bonding in metal-organic structures
NORM M. TUBMAN[1], JONATHAN L. DUBOIS, RANDOLPH Q. HOOD, SEBASTIEN HAMEL, ERIC R. SCHWEGLER, Lawrence Livermore National Laboratory — Transition metal sites in metal-organic frameworks and in doped carbon structures are actively being studied for their binding properties of molecular hydrogen. We present a study of prototypical metal-organic structures that can be used to bind molecular hydrogen non-covalently. Due to the well known limitations of current density functional theory based descriptions of non-covalent hydrogen bonding we have focused our efforts on a consistent many-body approach based on the fixed-node diffusion Monte Carlo method. Accurate studies of binding energies and the effects of multiple hydrogens in these structures are presented. Prepared by LLNL under Contract DE-AC52-07NA27344

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