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**Characterization of Hydrogen Interactions with $\delta$-Pu using Electronic Structure Theory**[1] CHRISTOPHER D. TAYLOR, Los Alamos National Laboratory, SARAH C. HERNANDEZ, University of Texas at Arlington — The generalized gradient approximation to density functional theory was used to study surface, bulk, defect, and reaction states of hydrogen in $\delta$-Pu. The quasi-disordered antiferromagnetic arrangement gave a volume of 24.1 Å$^3$ and a bulk modulus of 48.1 GPa for $\delta$-Pu, in reasonable agreement with the experimental values of 24.9 Å$^3$ and 30-35 GPa. This arrangement was thus subsequently used for all calculations. We have determined that hydrogen interactions with $\delta$-Pu are exothermic in character at all levels ranging from dissociative chemisorption to interstitial absorption, the formation of hydrogen-vacancy complexes, and generation of a hydride phase. The exothermic character of these interactions appears to be the reason for the rapid hydriding reaction, which has been determined experimentally to be essentially a barrierless process. The anionic character is observed to be retained. Our studies also indicate that vacancies do not appear to be strong traps for hydrogen, since the interstitial absorption sites are exothermic in nature. We will propose a scheme by which hydrogen interacts with Pu. Results will be compared with previous studies in the literature where available.

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