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Ab initio study on microscopic properties of III-V/water interfaces for photoelectrochemical hydrogen production BRANDON WOOD, WOON IH CHOI, ERIC SCHWEGLER, TADASHI OGITSU, LLNL — Photoelectrodes made of III-V semiconductors are known to exhibit very high solar-to-hydrogen conversion efficiency (from solar energy to chemical energy as H_2 bond); however, photocorrosion of the electrode in electrolyte solution remains an issue. Based on ab-initio molecular dynamics simulations, we study the structure, stability, and chemical activity of GaP/InP(001) semiconductor electrodes in contact with water. We will show how surface oxygen and hydroxyl change the electronic and chemical properties of water at the interface, leading to the formation of a strong hydrogen-bond network where fast surface hydrogen transport seems to be realized. Implications from our findings will be discussed in detail at the presentation. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52- 07NA27344.

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