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A first-principles investigation of III-V semiconductor-water interfaces for solar hydrogen production BRANDON WOOD, TADASHI OGITSU, ERIC SCHWEGLER, LLNL — Photoelectrochemical devices promise sustainable hydrogen production using sunlight and water. Currently, the highest efficiency devices use III-V semiconductor photoelectrodes; however, stability of these materials under operating conditions remains an issue. In an effort to understand the chemical properties of the electrode-water interface, we have performed first-principles molecular dynamics simulations on model III-V surfaces in realistic aqueous environments. The structure, stability, and chemical activity of these surfaces are investigated, with the aim of understanding the reactive states precursory to photoexcitation and hydrogen evolution. Our results show that surface oxide nucleation is key to facilitating surface reactivity, and that the surface oxygen bonding arrangement is important for determining of the available pathways for water dissociation and corrosion. This points to the importance of III-V surface oxides as intermediates in the water-dissociation component of hydrogen evolution. Prepared by LLNL under Contract DE-AC52-07NA27344.

Tadashi Ogitsu
LLNL

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