

Abstract Submitted
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First-principles study of III-V electrode interfaces for photoelectrochemical hydrogen production¹ BRANDON WOOD, TADASHI OGITSU, WOONI CHOI, ERIC SCHWEGLER, LLNL — Photoelectrochemical (PEC) cells promise clean, sustainable production of hydrogen fuel using water and sunlight. However, combining solar conversion efficiency with durability in electrolyte solution has proven difficult, in part because the complex chemistry active at the electrode-electrolyte interface remains poorly understood. We use first-principles molecular dynamics simulations and model density-functional calculations to study the structure, stability, and chemical activity of GaP/InP semiconductor electrodes in contact with water. We find that a local bond-topological model is able to capture much of the basic surface chemistry. Interpretation of our results points to the particular importance of surface-adsorbed oxygen in determining the available reaction pathways for photocorrosion and water dissociation. Electronic signatures of the local bond topologies are compared to data from X-ray absorption and emission spectroscopy for insight into actual electrode structure.

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