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Understanding performance and corrosion behavior of photo-electrode in terms of energetics of water-derived radicals on Ga-V (V=N,P,As) and GaP:N (110) surfaces: First-principles study WOON IH CHOI, JOHN TURNER, National Renewable Energy Laboratory, YONG-HYUN KIM, Korea Advanced Institute of Science and Technology, KWISEON KIM, National Renewable Energy Laboratory — Holes supplied from sunlight will detach the hydrogen atoms of H_2O as protons, leaving energetic O, H, or OH radicals. Therefore energetics of water-derived radicals on photo-electrode surface is important factor which determine its performance. Based on first-principles electronic structure and total energy calculations, we have studied reactions of -H, -O and -OH on the (110) surface of photo-cathode Ga-V and GaP:N materials, where V is N, P, and As. Zero-point energy and chemical potential of H_2 and O_2 gases are considered after static calculations. We have found that atomic oxygen on the GaN surface prefers being detached as O_2 to forming Ga-O. On the other hand, GaP and GaAs surfaces can have a strong Ga-O bond, hindering formation of O_2 gas and thus promoting surface corrosion. On GaP and GaAs surfaces hydrogen easily evolves as H_2 gas but on GaN not. Doped nitrogen in GaP to improve corrosion resistivity are tend to be clustered specially on the outermost surface region. These surface nitrogen atoms are expected to protect the surface and at the same time reduce hydrogen evolution rate.

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