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【504】pH-dependent surface chemistry and catalytic reaction pathway from first-principles

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We present a theoretical formulation for studying the pH-dependent interfacial coverage of semiconductor-water interfaces through ab initio electronic-structure calculations, molecular dynamics simulations, and the thermodynamic integration method. The proposed method is applied to study the BiVO₄(010)-water interface and yields a pH at the point of zero charge in excellent agreement with the experimental characterization. Furthermore, from the calculated pK_a values of the individual adsorption sites, we construct an ab initio concentration diagram of all the adsorbed species at the interface as a function of the pH of the aqueous solution. The achieved results are used in conjunction with the band alignment at the BiVO₄(010)-water interface, in order to study the pH-dependent catalytic reaction pathway for water splitting.

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