Nano Innovation 2024 Rome, 9-13 September
Conference & Exhibition

Manipulating the surface electronic properties of Si by molecular engineering for water splitting

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Abstract

The termination of surface-dangling bonds on silicon through Si–x bonds (x = C, or H), can reduce surface states in the electronic bandgap, thus altering electronic properties. Through a comprehensive study of doping levels (10^{14}–10^{20} cm^{-3}) and types (n and p), a consistent surface dipole trend induced by Si–H termination (the intial step to achive Si–C bonds) is discovered. It is achieved by redistributing surface charges and establishing thermal equilibrium with the chemical bond. This finding is further validated through ab initio simulations. To this end, we terminated the p-Si (111) with Si-C bonds to acheive efficient charge transfer between the silicon and the electrolyate for water splitting appications. This finding has immense implications not only for eliminating electronic defects at semiconductor interfaces, which is crucial in microelectronics but also for developing and engineering hybrid interfaces and heterojunctions with controlled electronic properties.