Diversity of Pt-sites at Pt/C₆₀ interface accelerates alkaline hydrogen evolution

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Alkaline Hydrogen Evolution Reaction (HER) is emerging as a focal point for sustainable hydrogen development as an alternative clean fuel. However, this method suffers from sluggish kinetics due to the additional water dissociation step. Here, we show that the activity of Pt towards alkaline HER can be significantly enhanced by anchoring ultra-small Pt nanoparticles (NPs) onto a fullerene (011) surface with unusually large lattice distance (~0.8 nm). This leads to a strong confinement of Pt NPs culminating into significant charge redistribution as observed in the charge distribution analysis. The binding energies of H and H₂O species were calculated to vary 0.28 eV and 0.5 eV more among Pt sites at the Pt(NP)/C₆₀ interface as compared to unsupported Pt NP. This profound difference suggests much more heterogeneous properties (in terms of binding strength towards key reaction intermediates) for Pt sites compared with Pt₁₄₀/C₆₀ interface. As a result, some of the interface sites exhibit low activation energies for Volmer and water dissociation steps, whereas other sites on the interface have low activation energies for Heyrovsky or Tafel steps. Detailed kinetic and computational investigations revealed the origin of the enhanced activity to be the diverse binding properties of the Pt-sites at the interface of Pt/C_{60} (011), which generates highly active sites for all elementary steps in alkaline HER, particularly the sluggish Volmer and water dissociation step as compared to unsupported Pt particles and state of art Pt/C catalyst.