

Supporting Information

A Novel Metal-free Two-Dimensional Material for Photocatalytic Water Splitting ----- Phosphorus Nitride (γ -PN)

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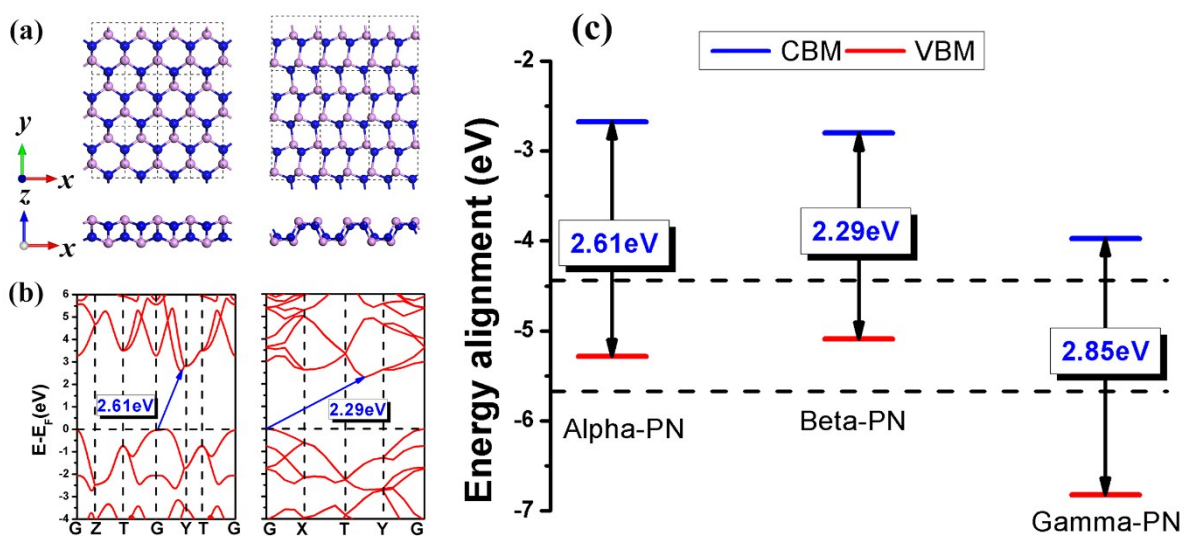


Figure S1. (a) The top view and side view of α - and β -PN nanosheet and (b) the corresponding band structure. (c) The energy level alignment comparison among three types of phosphorus nitride nanosheet relative the vacuum level.

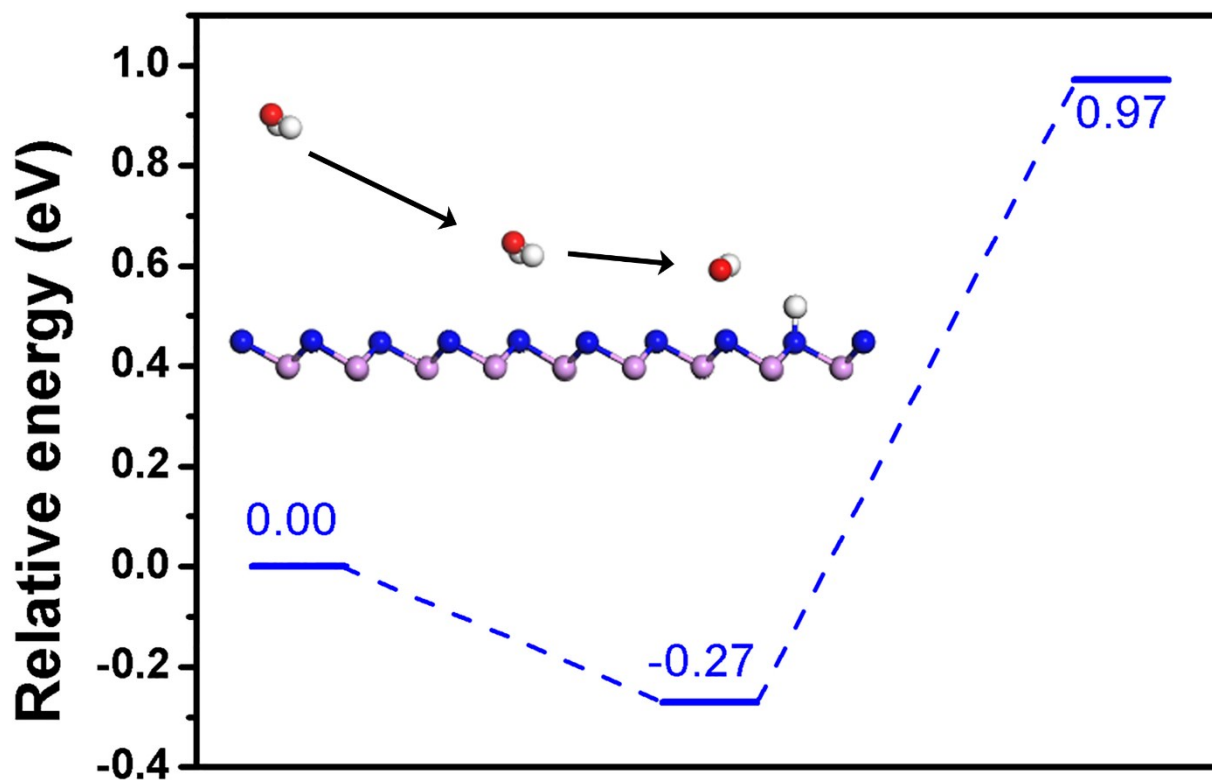


Figure S2. The water decomposition mechanism of H_2O on 2D γ -PN monolayer.