Supplementary Information
Theoretical Investigation on BeN$_2$ Monolayer for an Efficient Bifunctional Water Splitting Catalyst

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Figure S1: Dispersion of phonon modes of the BeN$_2$ monolayer calculated with $3\times3\times1$ supercell.
Figure S2: Total energy fluctuation during AIMD simulations at 300 K and the insets are snapshot structures of the BeN\textsubscript{2} monolayer at 0 ps and 10 ps.
Figure S3: Computationally predicted Pourbaix diagram of BeN$_2$ system. The stable phases include ion phase Be(s) and BeO(s). The orange dashed lines denote potentials of 0 V vs RHE and 1.23 V vs RHE.

Figure S4: Calculated band structure and density of states of BeN$_2$ monolayer obtained from PBE and band structure using HSE06 functional are shown in (a) and (b), respectively. The Fermi level is set to zero. (c) Calculated band edge positions of BeN$_2$ monolayer with respect to vacuum potential. The dashed lines are water redox potentials at pH = 0.
Figure S5: Iso-surface plot of charge density difference between BeN$_2$ monolayer and reaction intermediates (a) *O, (b) *OH, (c) *OOH, (d) *H, (e) *H$_2$O, and (f) *H$_3$O. The isosurface value is set to be 0.015 Å$^{-3}$. The color yellow (cyan) represents an accumulation (loss) of electrons.