Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Preparation of TiO_xN_y/TiN Composite for Photocatalytic Hydrogen Evolution under Visible Light

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Table S1 Calculation conditions for geometry optimization and energy task

Task: Geometry optimization			Energy
Functional	GGA[1,2] PW91[3]		LDA CA-PZ [4,5]
Minimizer	Fine quality		-
	Energy:	1.0e-5 eV/atom	-
	Max force:	0.03 eV/	-
	Max stress:	0.05 GPa	-
	Max displacement:	0.001 Å	-
Algorithm	BFGS[6]	use line search	-
Stress	0 for all		-
Energy cutoff	700 eV		700 eV
SCF tolerance	$1.0*10^{-6}$ eV/atom		$1.0*10^{-6}$ eV/atom
Pseudopotentials	Ultrasoft [7]		Norm-conserving [8]
FFT grid density	Fine quality		Standard
Finite basis correction	Smart		Smart
Electronic minimizer	Density Mixing[9]		Density Mixing[9]
Orbital occupancy	Fixed		Fixed
k point quality	Fine quality		Fine quality
Band structure	Unchecked		Checked Fine quality k point set
Density of states	Unchecked		Checked Medium quality k point set

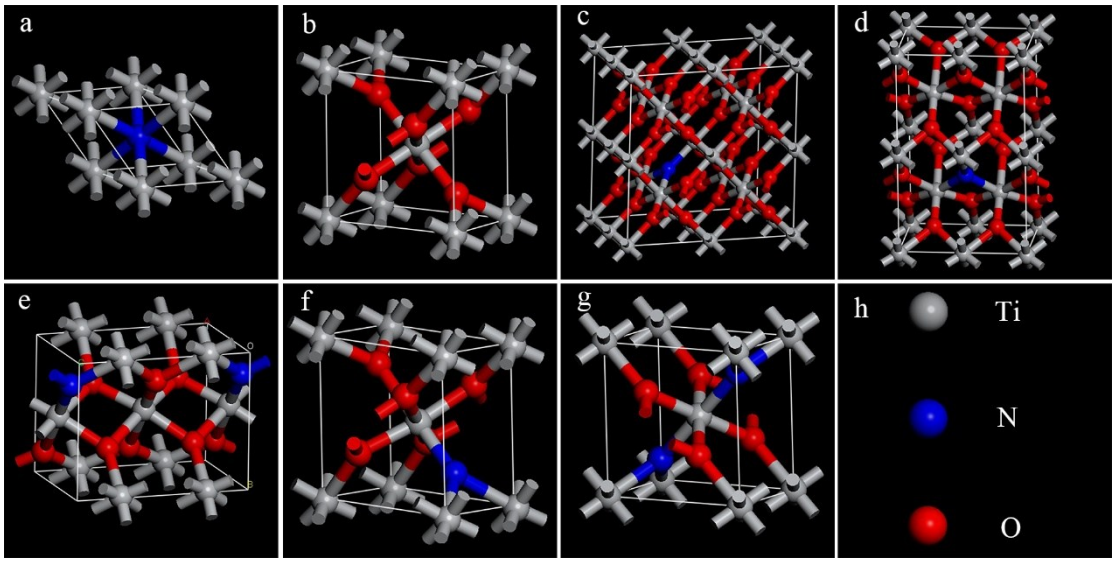

Fig. S1. Structures of calculation models

Table S2 The lattice parameter and grain size of the nitridation products at different temperature with 3 h

Temperature (°C)	800	850	900	950	1000	JCPDS card 38-1420
a (nm)	0.4216	0.4228	0.4237	0.4241	0.4241	0.4241
Grain size (nm)	35.5±1.5	36.1±1.9	37.0±1.6	37.9±1.7	38.5±2.4	

Table S3 The lattice parameter and grain size of the nitridation products with different time at 900 °C

Time(h)	2	3	4	5	JCPDS card 38-1420
a (nm)	0.4233	0.4236	0.4238	0.4241	0.4241
Grain size (nm)	35.2±1.3	36.8±2.2	37.2±1.4	38.3±0.7	

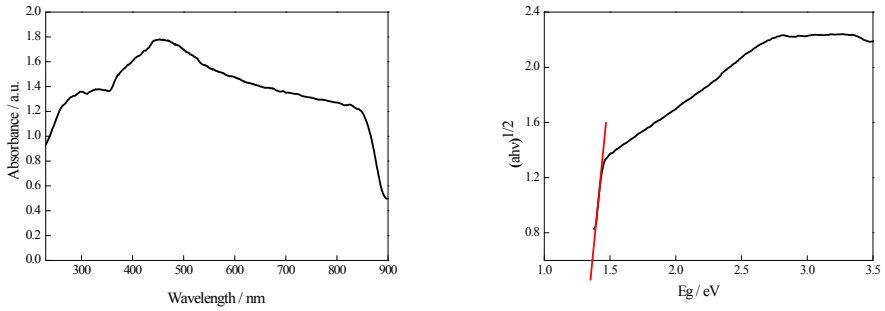

Fig. S2. (a) UV-vis diffuse reflection spectra of yolk–shell TiO_xN_y/TiN, (b) The plots of $(\alpha h\nu)^{1/2}$ versus hν. The bandgap of yolk–shell TiO_xN_y/TiN.

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