Electronic Supporting Information

B-doped 3C-SiC nanowires with finned microstructure for efficient visible-light-driven photocatalytic hydrogen production

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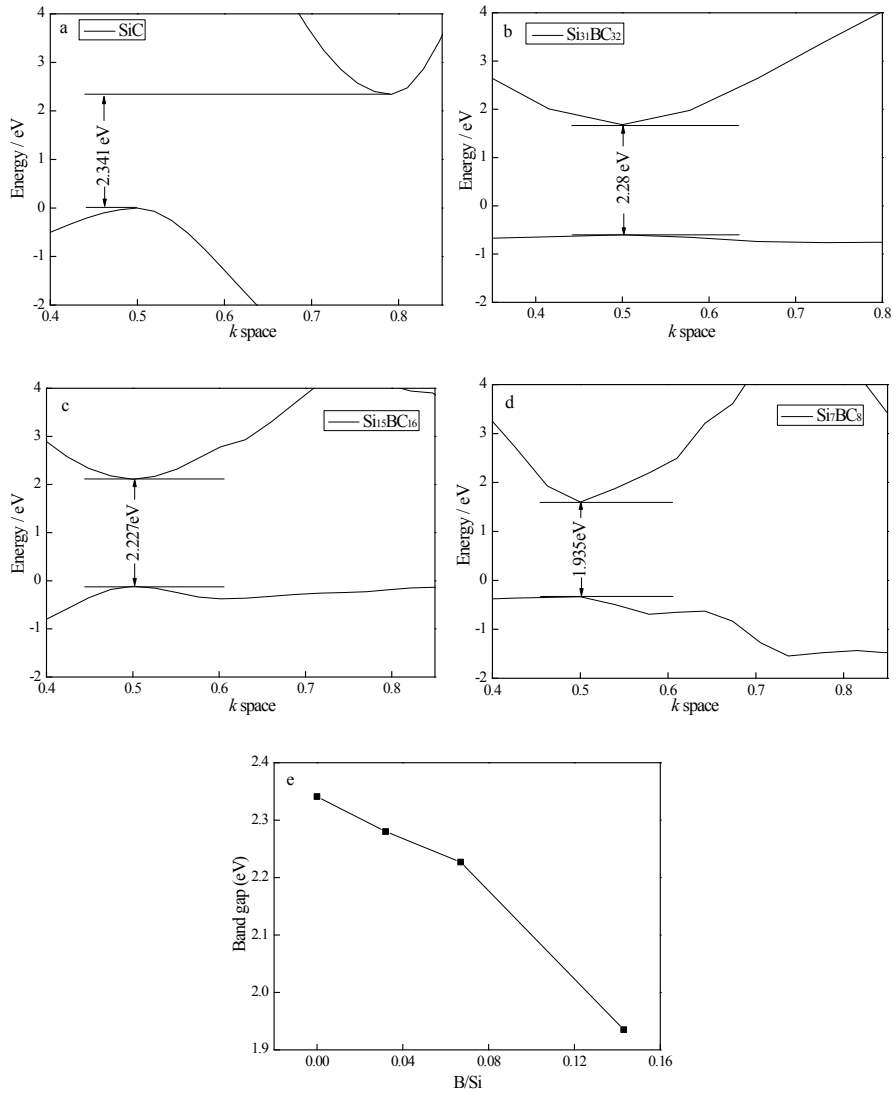
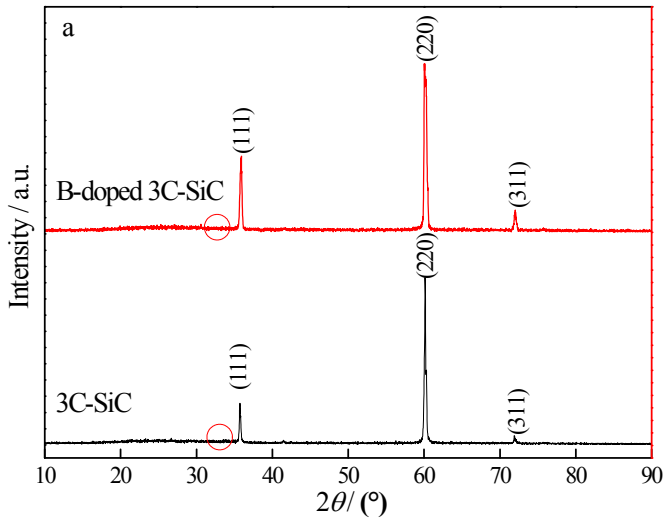


Fig. S1 (a)-(d) Calculated PDOS of 3C-SiC and B-doped 3C-SiC including $Si_{31}BC_{32}$, $Si_{15}BC_{16}$ and Si_7BC_8, (e) is the band gap of $Si_{n-1}BC_n$ (n=8, 16, 32).



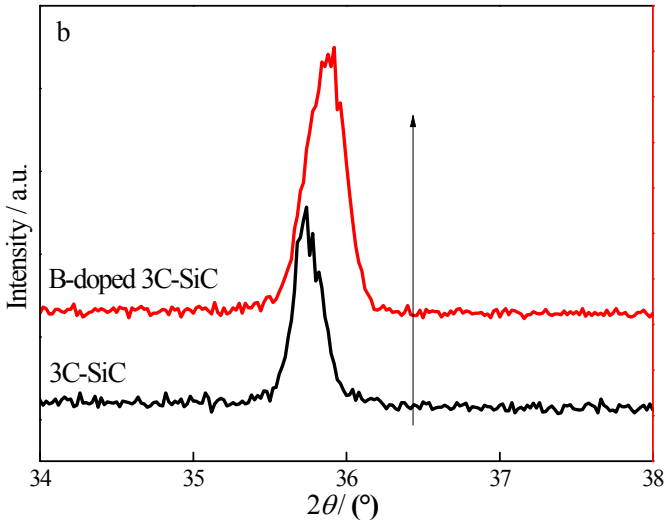
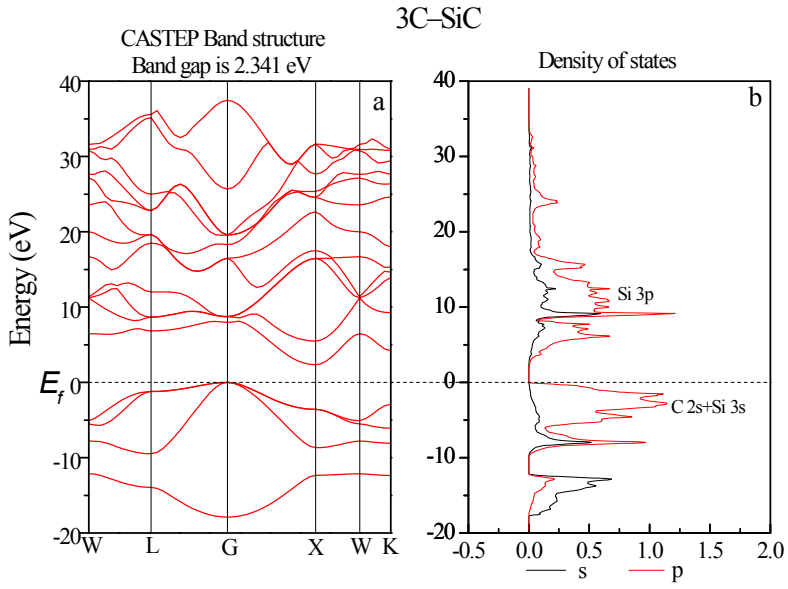


Fig. S2. XRD patterns of the as-prepared (a) and the magnification of the diffraction peak (111) (b)



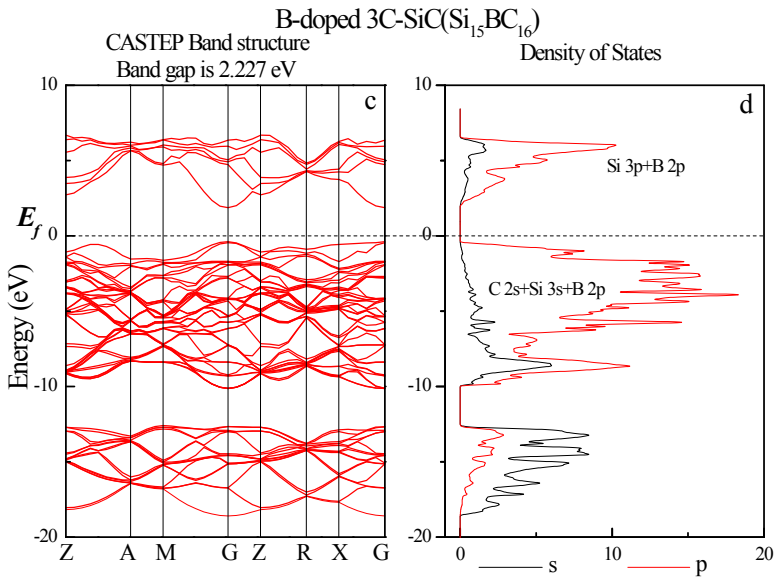
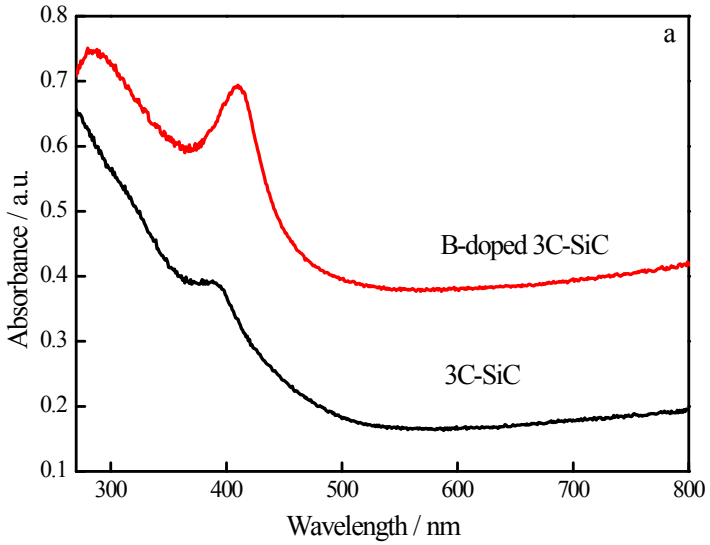


Fig. S3. The calculated energy band and density of states (DOS) of pure 3C-SiC (a and b) and B-doped 3C-SiC (c and d)



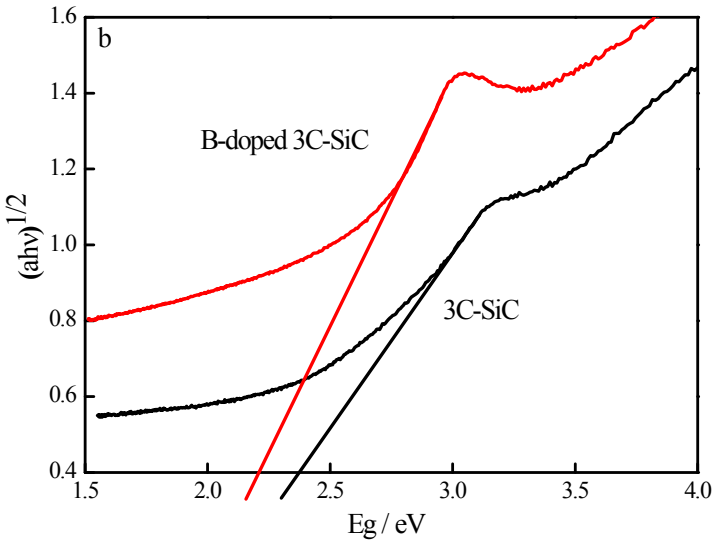


Fig. S4. (a) UV-Vis diffusion reflectance spectra (b) The plots of $(\alpha hv)^{1/2}$ versus hv. The bandgap of the samples

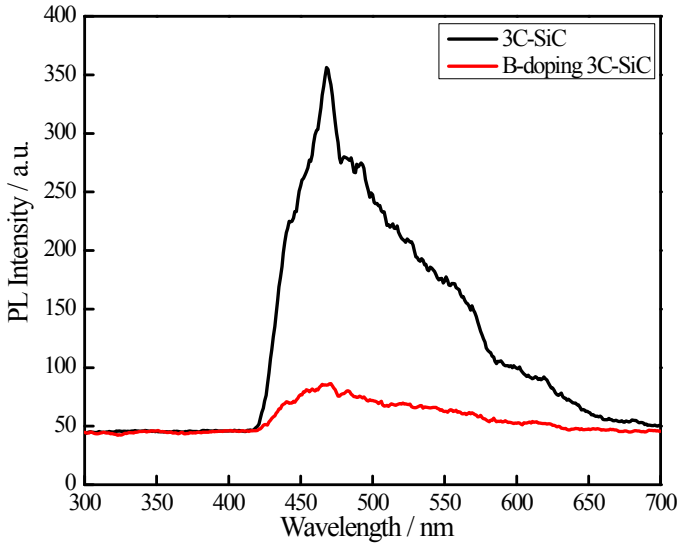


Fig. S5 Photoluminescence spectra of 3C-SiC and B-doped 3C-SiC.

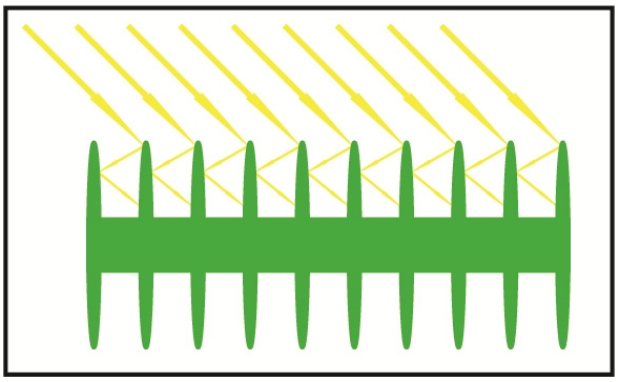
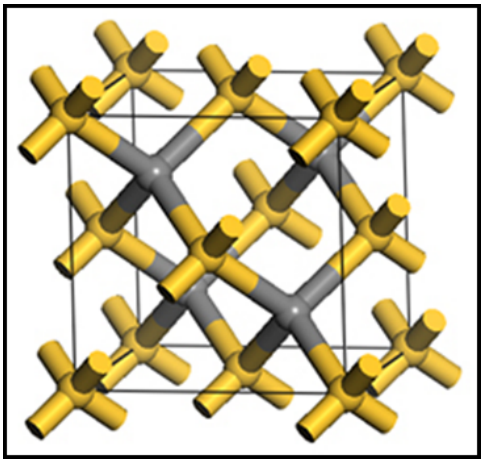


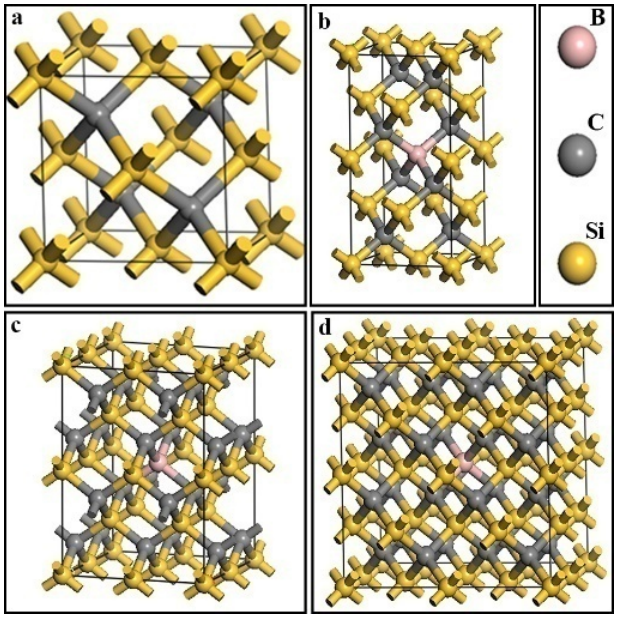
Fig. S6 Light reflection models in the B-doped 3C-SiC nanowires.

Table S1 Calculation conditions for geometry optimization and energy task

Task: Geometry optimization			Energy	
Functional	GGA PW91		LDA CA-PZ[1,2]	
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:	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[3]		Norm-conserving[4]	
FFT grid density	Fine quality		Standard	
Finite basis correction	Smart		Smart	
Electronic minimizer	Density Mixing		Density Mixing	
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



Scheme 1. 3C-SiC with a zinc blende structure



Scheme 2. Structures of calculation models

References

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