Electronic Supplementary Material (ESI) for Environmental Science: Advances.

Supporting information

Crystal phase engineering SiC nanosheet for enhancing photocatalytic CO_2 reduction

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Table S1. The Raman peak area ratio of SiC-0, SiC-0.2, SiC-P0.3, SiC-0.5, SiC-0.8.

PVP dosing quantity	0 g	0.2 g	0.3 g	0.5 g	0.8 g
Ratio*	0	0.2776	0.4674	0.3017	0.2628

* The ratio of the Raman peak area of the TA characteristic peak for 2H phase to the TO characteristic peak for 3C phase SiC.

Table S2. The optical absorption band edge and energy band gap of SiC-0, SiC-0.2, SiC-P0.3, SiC-0.5, SiC-0.8.

Sample	Optical absorption band edge / nm	Optical energy band gap / eV
SiC-0	507	2.45
SiC-0.2	488	2.54
SiC-0.3	470	2.64
SiC-0.5	481	2.57
SiC-0.8	492	2.52

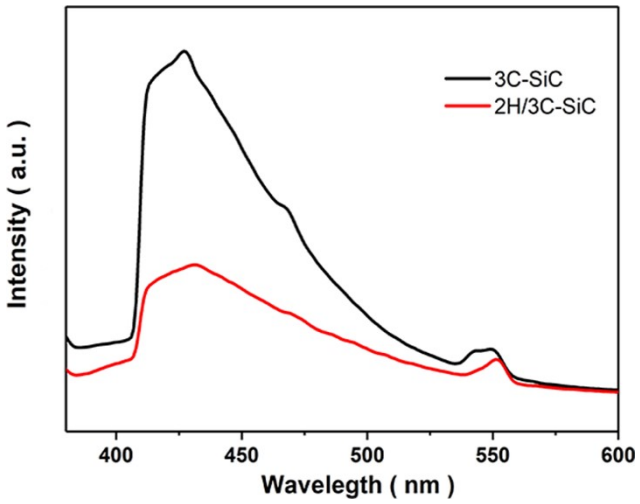

Figure S1. The steady-state photoluminescence spectra for 3C SiC and 2H/3C SiC.

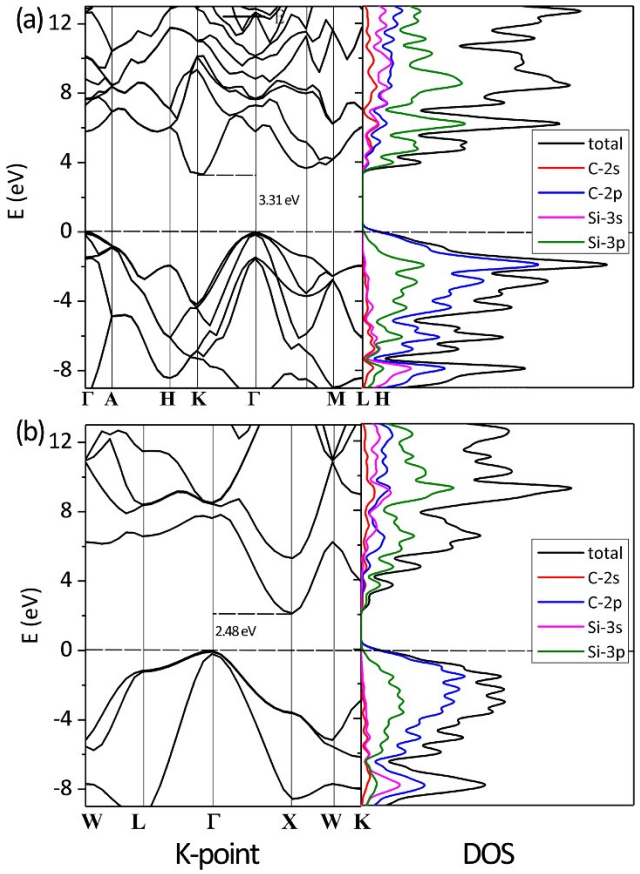

Figure S2. The band structure and density of states (DOS) for (a) 2H SiC and (b) 3C SiC.

The theoretical calculation is based on the generalized gradient approximation (GGA)[1] and the PBE[2] exchange correlation function, and the density functional calculation of the local configuration relaxation and electronic structure is performed by CASTEP[3]. The $2s^2 2p^2$ of C and the $3s^2 3p^2$ of Si

are the corresponding valence electrons. Since conventional DFT methods often underestimate the energy gap, the shielded exchange hybrid density functional (HSE06) method[4] was used to correct the energy gap of PBE. The cutoff energy of the plane wave basis set is 500 eV. A suitable Monkhorst-Pack K-point grid was employed to keep the enthalpy convergence up to 10^{-6} eV. During configuration optimization, K-point grids of 5 × 5 × 5 and 7 × 7 × 2 were used for the 3C and 2H phases, respectively, and all atoms were allowed to relax until the atomic forces were less than 0.02 eV/Å.

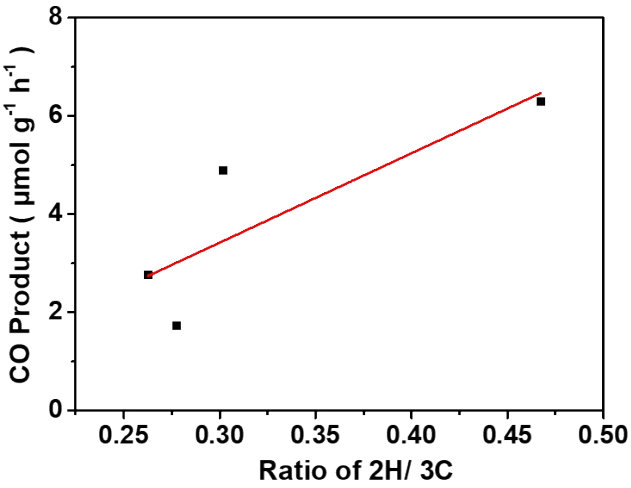

Figure S3. CO product on the SiC samples with different ratio of 2H and 3C.

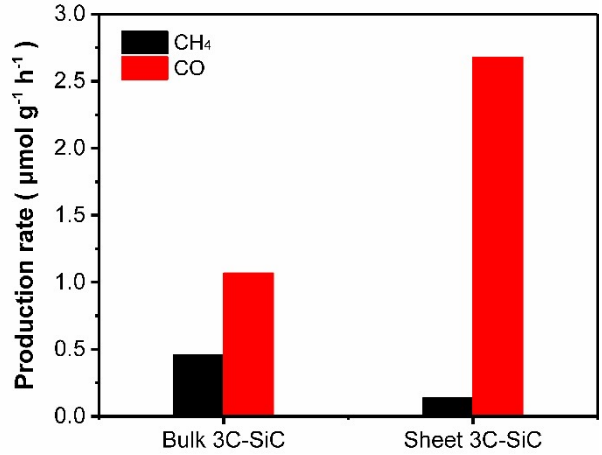

Figure S4. CH_4 and CO production rate on the bulk 3C-SiC and sheet 3C-SiC samples.

References

1. J. P. Perdew and Y. Wang, Accurate and simple analytic representation of the electron-gas correlation energy, *Physical review B*, 1992, **45**, 13244.
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3. S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson and M. C. Payne, First principles methods using CASTEP, *Zeitschrift für kristallographie-crystalline materials*, 2005, **220**, 567-570.
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