## **Electronic Supplementary Information**

## InNi $_{3}C_{0.5}$ (a)C-derived InNi $_{3}$ alloy as a coke-resistant low-temperature catalyst for selective butadiene hydrogenation

Zhibing Chen,<sup>+</sup> <sup>a</sup> Yali Lv,<sup>+a,b</sup> Xintai Chen,<sup>a</sup> Xiaoling Mou,<sup>\*a,c</sup> Jingwei Li,<sup>\*b</sup> Li Yan,<sup>b</sup> Ronghe Lin, <sup>\*a,c</sup> and Yunjie Ding<sup>\*a,b,d</sup>

<sup>a</sup>Hangzhou Institute of Advanced Studies, Zhejiang Normal University, 1108 Gengwen Road, Hangzhou 116023, PR China. xiaoling.mou@zjnu.edu.cn, catalysis.lin@zjnu.edu.cn.

<sup>b</sup>Dalian National Laboratory for Clean Energy, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, China. dyj@dicp.ac.cn.

<sup>c</sup>Key Laboratory of the Ministry of Education for Advanced Catalysis Materials, Zhejiang Normal University, 688 Yingbin Road, Jinhua 321004, China.

<sup>d</sup>The State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, 457 Zhongshan Road, Dalian 116023, China.

<sup>+</sup> Equal contribution.

\*Corresponding authors. E-mails: xiaoling.mou@zjnu.edu.cn, lijw@dicp.ac.cn, catalysis.lin@zjnu.edu.cn, dyj@dicp.ac.cn.

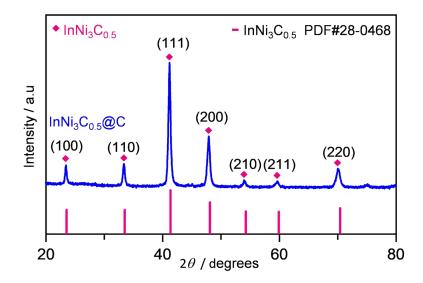
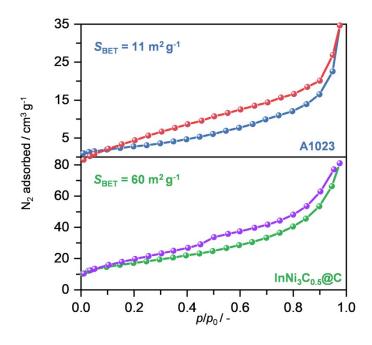
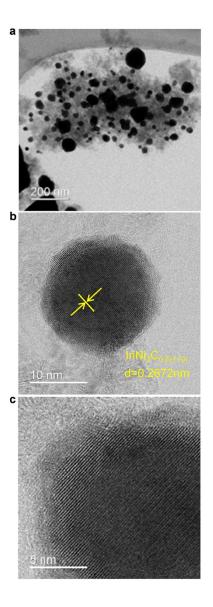


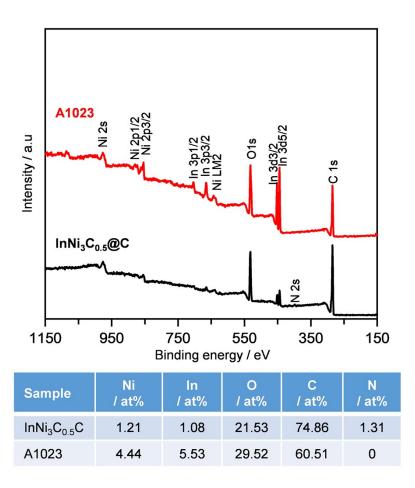
Fig. S1. The PXRD patterns of the as-prepared  $InNi_3C_{0.5}@C$ .



**Fig. S2.** The  $N_2$  sorption isotherms of pristine In $Ni_3C_{0.5}$ @C and A1023.



**Fig. S3.** The STEM images H1023, showing the reduced carbon shells after hydrogenation treatment at 1023 K.



**Fig. S4.** The full XPS spectra of  $InNi_3C_{0.5}@C$  and A1023 (oxidized at 1023 K), accompanied with the elemental distribution.

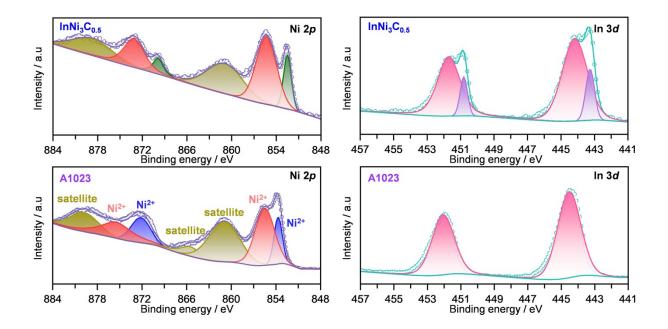


Fig. S5. The Ni 2p and In 3d XPS spectra of InNi<sub>3</sub>C<sub>0.5</sub>@C and A1023 (oxidized at 1023 K).

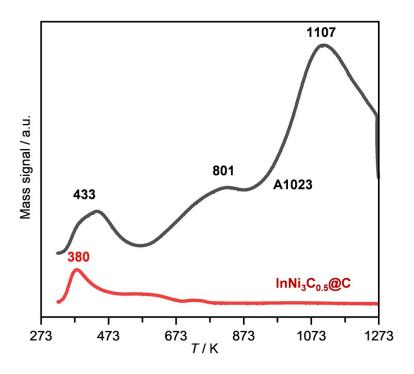
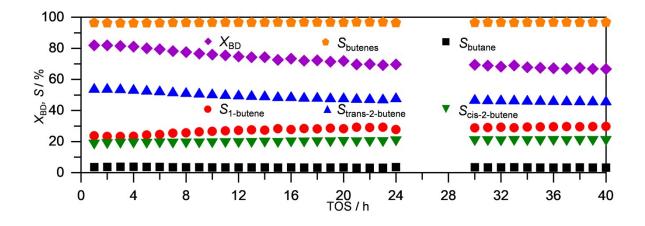


Fig. S6. The mass signals (m/z = 2) during the H<sub>2</sub>-TPD experiments on  $InNi_3C_{0.5}@C$  and A1023.



**Fig. S7.** The stability performance of A1023 in BD hydrogenation. Reaction conditions: 0.69 vol.% BD balanced in N<sub>2</sub>, H<sub>2</sub>:BD = 50, *GHSV* = 300,000 cm<sup>3</sup> g<sub>cat</sub><sup>-1</sup> h<sup>-1</sup>, *T* = 353 K.

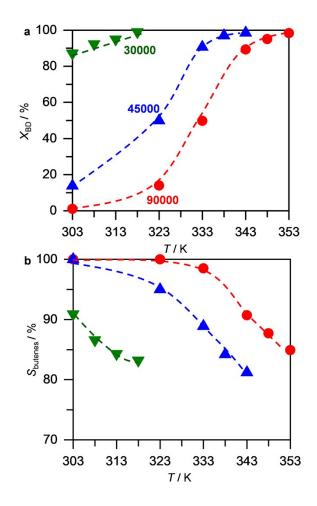


Fig. S8. The **a**, BD conversion and, **b**, product selectivity as a function of temperature in BD hydrogenation on A1023. Reaction conditions: 0.69 vol.% BD balanced in N<sub>2</sub>, H<sub>2</sub>:BD = 50,  $GHSV = 300,000-900,000 \text{ cm}^3 \text{ g}_{cat}^{-1} \text{ h}^{-1}$ .

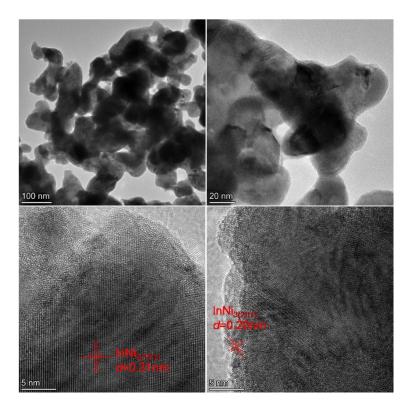


Fig. S9. The TEM images at different magnifications of A1023 after the 24 h evaluation in BD hydrogenation. The distinct (101) and (201) facets of  $InNi_3$  alloy were evidenced from the high-resolution TEM images.

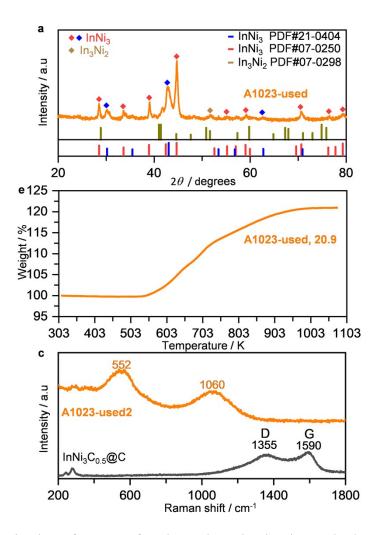


Fig. S10. Characterization of A1023 after the 36 h evaluation in BD hydrogenation at 318 K:a, PXRD; b, TGA; c, Raman spectra.