Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics. This journal is © the Owner Societies 2024

## **Supplementary Information**

## Enhanced As-COF nanochannels as a high-capacity anode for K and Ca-ion batteries

Shehzad Ahmed <sup>a</sup>, Awais Ghani <sup>b</sup>, Imran Muhammad <sup>c</sup>, Iltaf Muhammad <sup>a</sup>, Andleeb Mehmood <sup>a</sup>, Naeem Ullah <sup>a</sup>, Arzoo Hassan <sup>a</sup>, Yong Wang <sup>d</sup>, Tian Xiaoqing <sup>a\*</sup> and Boris Yakobson <sup>e</sup>

<sup>a</sup> College of Physics and Optoelectronic Engineering, Shenzhen University, Guangdong 518060, P. R China.

<sup>b</sup> Smart Materials for Architecture Research Lab, Innovation Center of Yangtze River Delta, Zhejiang University, Jiaxing 314100, P. R China

<sup>c</sup> Department of Chemistry and Guangdong Provincial Key Laboratory of Catalytic Chemistry, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China

<sup>d</sup> School of Physics, Nankai University, Tianjin 300071, P. R China

<sup>e</sup> Department of Materials Science and Nano Engineering Department of Chemistry and the Smelly Institute for Nano Scale Science and Technology Rice University Houston, TX 77005, USA

Email: xqtian@szu.edu.cn

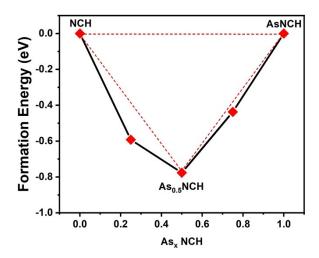


Fig. S1. Convex hull of the calculated  $E_{\rm f}\, versus$  As concentration for the As-COF.

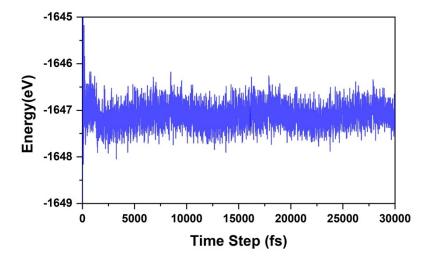


Fig. S2. Variations in total energy versus time for the As-COF in AIMD simulations of 30 ps at 300 K respectively.

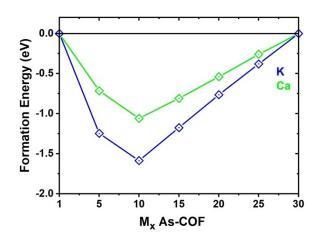


Fig. S3. Convex hull of the calculated  $E_{\rm f}$  versus K and Ca concentration for the As-COF.