

**Electronic Supplementary Information for**  
**Stable puckered C<sub>2</sub>N<sub>2</sub> nanosheet with giant anisotropic hole carrier mobility: insights**  
**from first-principles**

Yanli Wang<sup>1, a)</sup> and Yi Ding<sup>2, b)</sup>

<sup>1)</sup> *Department of Physics, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, People's Republic of China*

<sup>2)</sup> *Department of Physics, Hangzhou Normal University, Hangzhou, Zhejiang 311121, People's Republic of China*

Table S1: the hole mobility information of bp-C<sub>2</sub>N<sub>2</sub> nanosheet from the FHI-aims calculation.

---

<sup>a)</sup> wangyanli-04@tsinghua.org.cn

<sup>b)</sup> dingyi2001@tsinghua.org.cn

TABLE I. Calculated hole mobility data by the FHI-aims code for the bp-C<sub>2</sub>N<sub>2</sub> nanosheet.  $C$ ,  $m$ ,  $E$  and  $\mu$  are the elastic constant, effective mass, deformation potential constant and carrier mobility, respectively. The data in brackets are calculated by the HSE functional, which is also done with the FHI-aims code.

	$C$	$m$	$E$	$\mu$ ( $10^3\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ )	
	(N/m)	( $m_0$ )	(eV)	DPT formula (1)	DPT formula(2)
hole ( $x$ )	454	0.40 (0.41)	-0.018 (0.051)	22131 (5765)	1.52 (2.30)
hole ( $y$ )	681	18.64 (6.53)	-5.84 (-6.14)	0.008 (0.036)	0.016 (0.070)