

## Supplementary Materials for Giant magnetic anisotropy of two-dimensional metal–dicyanoanthracene framework

Yun Zhang<sup>1,2,3</sup>, Zhao Wei<sup>1</sup>, Meiguang Zhang<sup>1</sup>, Xiao Gu<sup>2, 4\*</sup>, Li Huang<sup>3\*</sup>

<sup>1</sup>*Department of Physics and Information Technology, Baoji University of Arts and Sciences, Baoji 721016, China*

<sup>2</sup>*Department of Applied Physics, Chongqing University, Chongqing 400044, P.R. China*

<sup>3</sup>*Department of Physics, Southern University of Science and Technology, Shenzhen, Guangdong 518055, China*

<sup>4</sup>*Faculty of Science, Ningbo University, Ningbo-315211, P.R. China*

### Supplementary computational methods

Table S1. Effective  $U$  value ( $U_{\text{eff}}$ ) versus the calculated MAE (in meV) of Ir-DCA.

$U_{\text{eff}}$ (eV)	0	0.5	1.0	1.5	2.0	SCAN
MAE(meV)	180	188.36	119.56	24.319	18.4	259

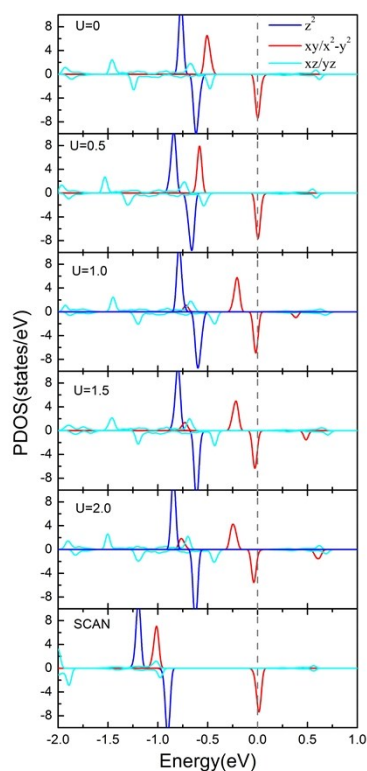


Fig. S1. Projected density of states (PDOS) of Ir-DCA

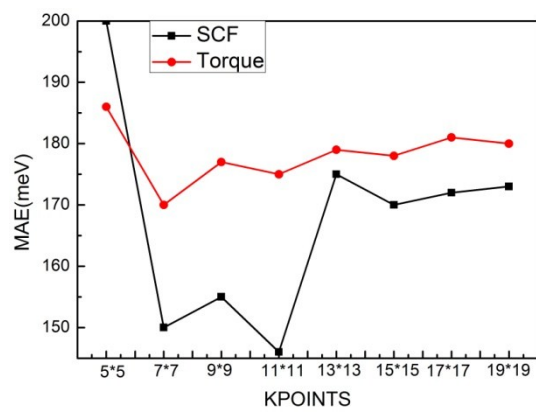


Fig. S2. K points convergences for torque and direct method, respectively.