

## Supplementary file

### Constructing trifunctional MoTe<sub>2</sub>/As van der Waals heterostructure for versatile energy applications

Yee Hui Robin Chang <sup>a, \*</sup>, Keat Hoe Yeoh <sup>b, c, \*</sup>, Junke Jiang <sup>d</sup>, Thong Leng Lim <sup>e</sup>, Yik Seng Yong <sup>e</sup>, Lay Chen Low <sup>e</sup>, Moi Hua Tuh <sup>f</sup>

<sup>a</sup> Faculty of Applied Sciences, Universiti Teknologi MARA, Cawangan Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia

<sup>b</sup> Department of Electrical and Electronic Engineering, Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, 43000 Kajang, Selangor, Malaysia

<sup>c</sup> Center for Photonics and Advanced Material Research, Lee Kong Chian Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, 43000 Kajang, Selangor, Malaysia

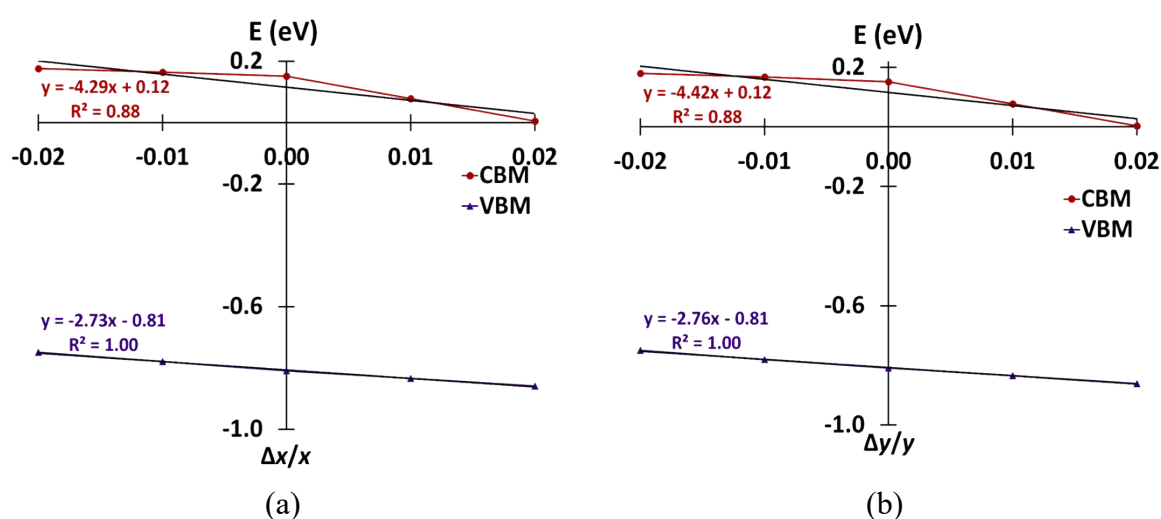
<sup>d</sup> Univ Rennes, ENSCR, CNRS, ISCR-UMR 6226, F-35000 Rennes, France

<sup>e</sup> Faculty of Engineering and Technology, Multimedia University, Jalan Ayer Keroh Lama, 75450 Melaka, Malaysia

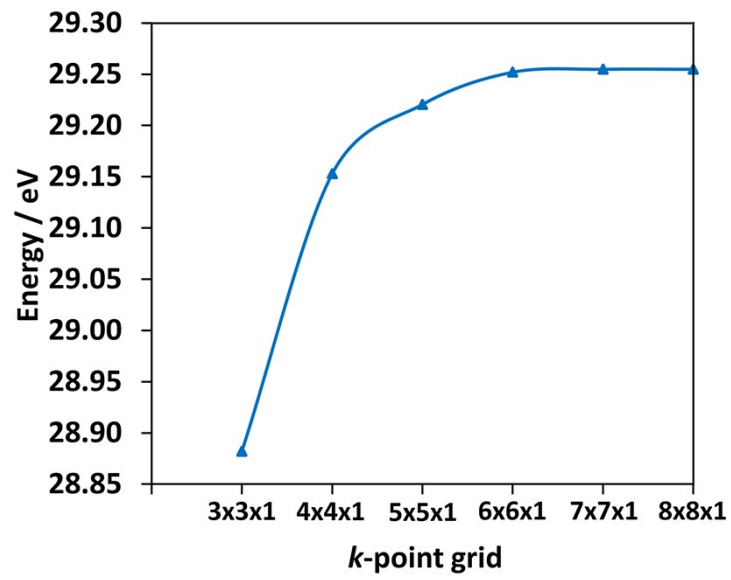
<sup>f</sup> Faculty of Computer & Mathematical Sciences, Universiti Teknologi MARA, Cawangan Sarawak, 94300 Kota Samarahan, Sarawak, Malaysia

\*Electronic mail: robincyh@uitm.edu.my; keathoe.yeoh@gmail.com

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**S1** Band energies of the CBM and VBM for MoTe<sub>2</sub>/As heterostructure as a function of lattice dilation along x and y directions. The fitted slopes show the  $E_D$  in eV.



S2  $k$ -points convergence test. For clarity, the  $y$ -axis is plotted in reverse.