Electronic Supplementary Information (ESI) for the manuscript:

Assessing the stability of Cd_3As_2 Dirac semimetal in humid environments: the influence of defects, steps and surface oxidation

Yanxue Zhang[1,§], Silvia Nappini[2,§], Raman Sankar[3], Federica Bondino[2,*], Junfeng Gao[1*], and Antonio Politano[4,5,*]

1 Laboratory of Materials Modification by Laser, Ion and Electron Beams, Dalian University of Technology, Ministry of Education, Dalian 116024, China

2 Consiglio Nazionale delle Ricerche (CNR)- Istituto Officina dei Materiali (IOM), Laboratorio TASC in Area Science Park S.S. 14 km 163.5 34149 Trieste, Italy
3 Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan
4 Department of Physical and Chemical Sciences, University of L'Aquila, via Vetoio, 67100 L'Aquila (AQ), Italy
5 CNR-IMM Istituto per la Microelettronica e Microsistemi, VIII strada 5, I-95121 Catania, Italy

§ These authors contributed equally

*corresponding authors: Federica Bondino (bondino@iom.cnr.it); Junfeng Gao (gaojf@dlut.edu.cn) and Antonio Politano (antonio.politano@univaq.it)

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S1. X-ray diffraction (XRD)

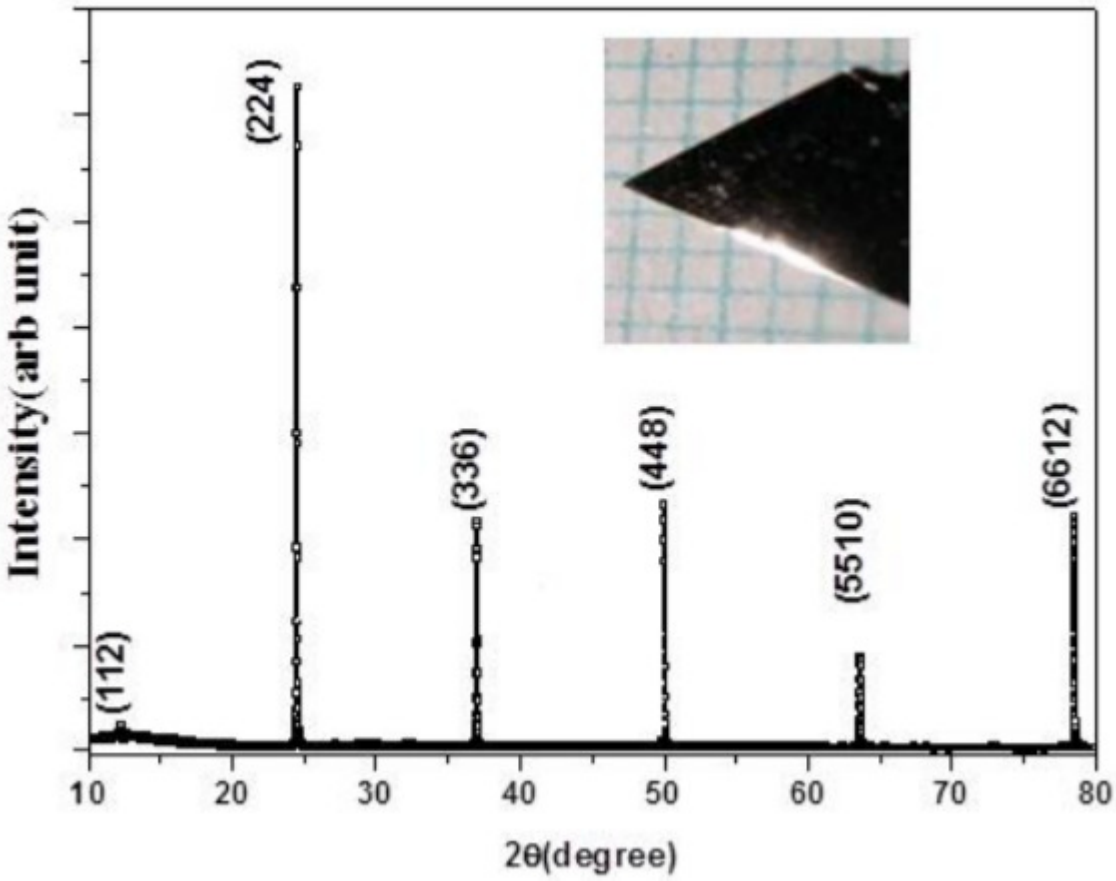

Figure S1. XRD pattern of (112)-oriented foils of Cd3As2

S2. X-Ray photoemission spectroscopy (XPS)

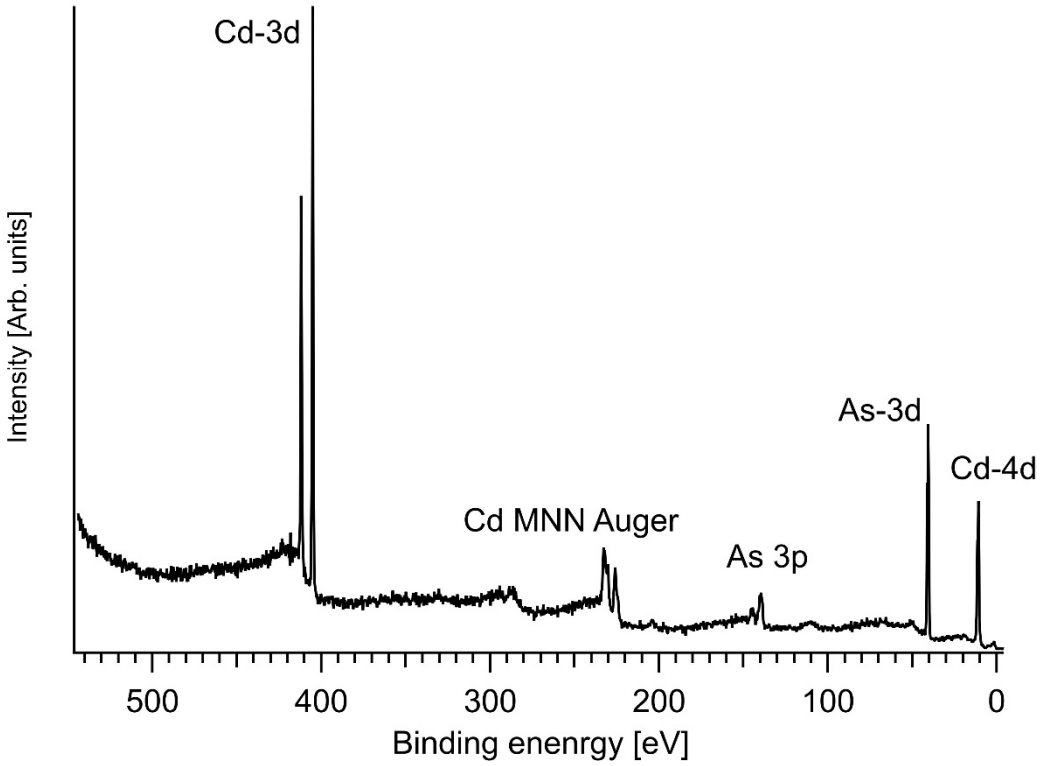

Figure S2. Survey spectrum of as-cleaved Cd_3As_2 measured with a photon energy of 610 eV. Notably, no relevant signal from O-1s and C-1s is recorded, thus demonstrating the surface cleanliness.

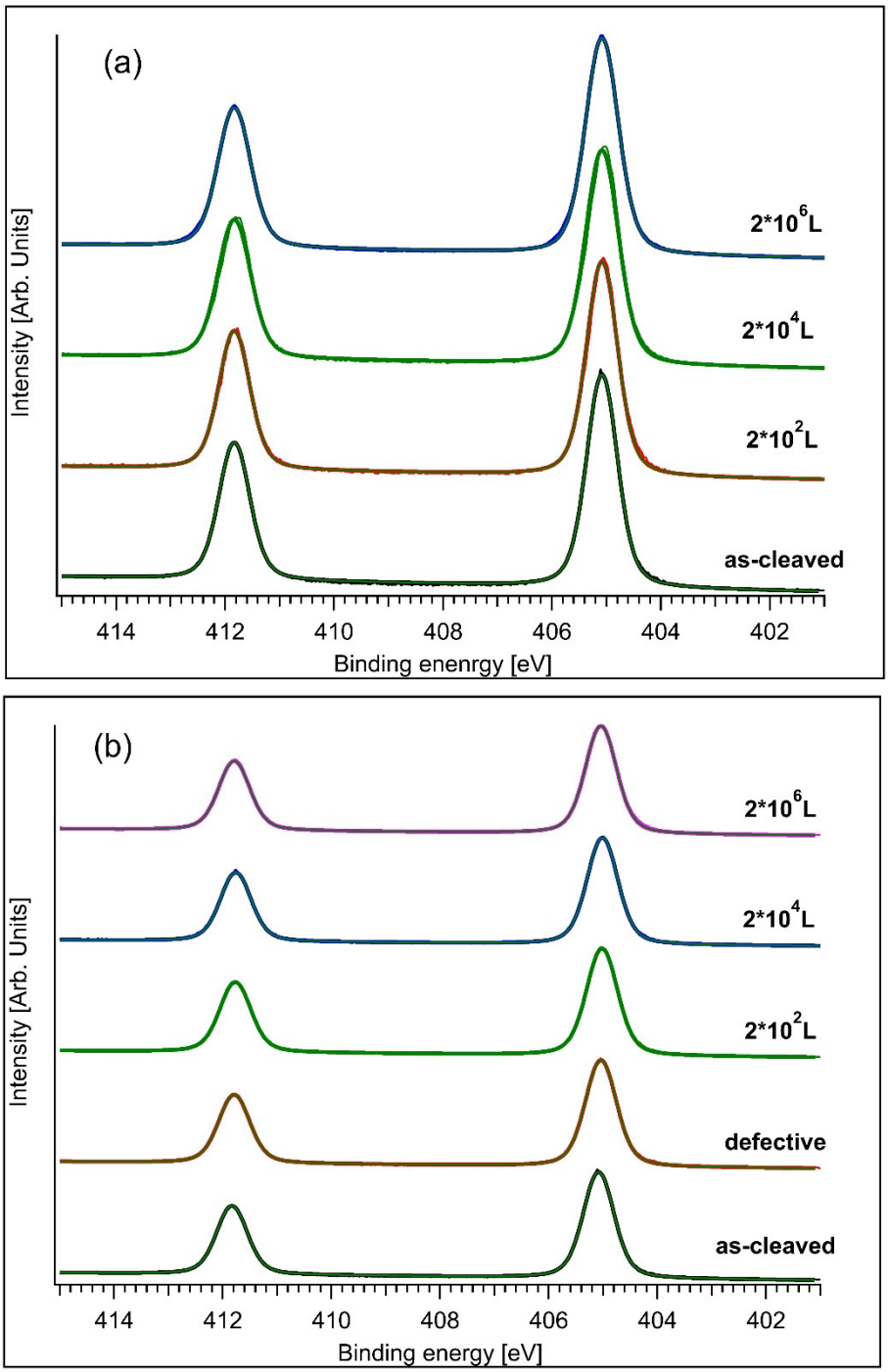

Figure S3. Cd-3d core-level for as-cleaved Cd_3As_2 (a) and defective Cd_3As_2 surfaces (b) exposed to 23 L, $2 \cdot 10^2$ L, $2.3 \cdot 10^4$ L and $1.1 \cdot 10^6$ L of H_2O. The incident photon energy is 596 eV.

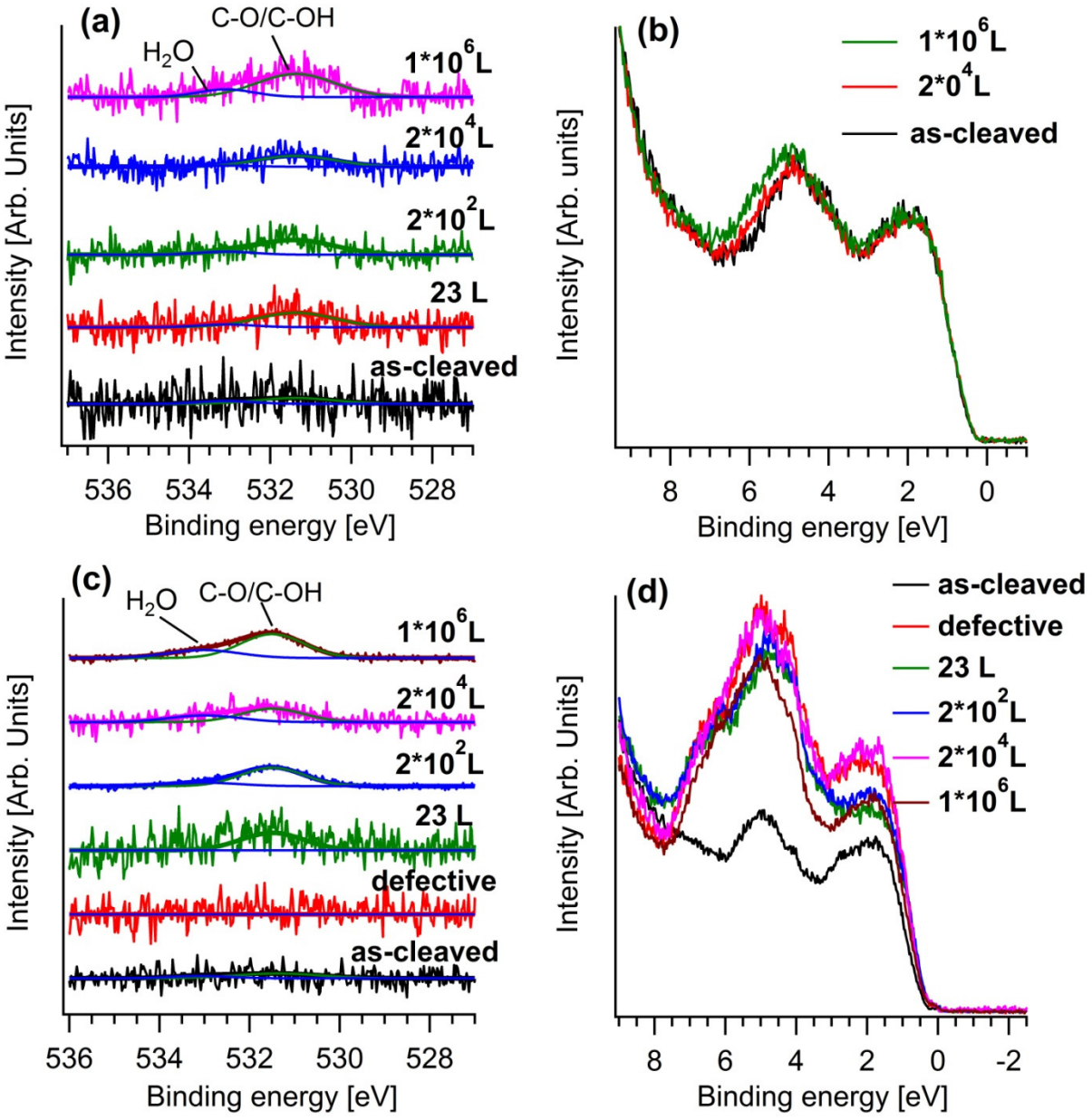

Figure S4. O-1s and valence band spectra for as-cleaved Cd_3As_2 (top) and defective Cd_3As_2 surfaces (bottom) exposed to 23 L, $2 \cdot 10^2$ L, $2.3 \cdot 10^4$ L and $1.1 \cdot 10^6$ L of H_2O. The incident photon energy used to measure O-1s is 596 eV, while the valence band was measured with a photon energy of 190 eV.

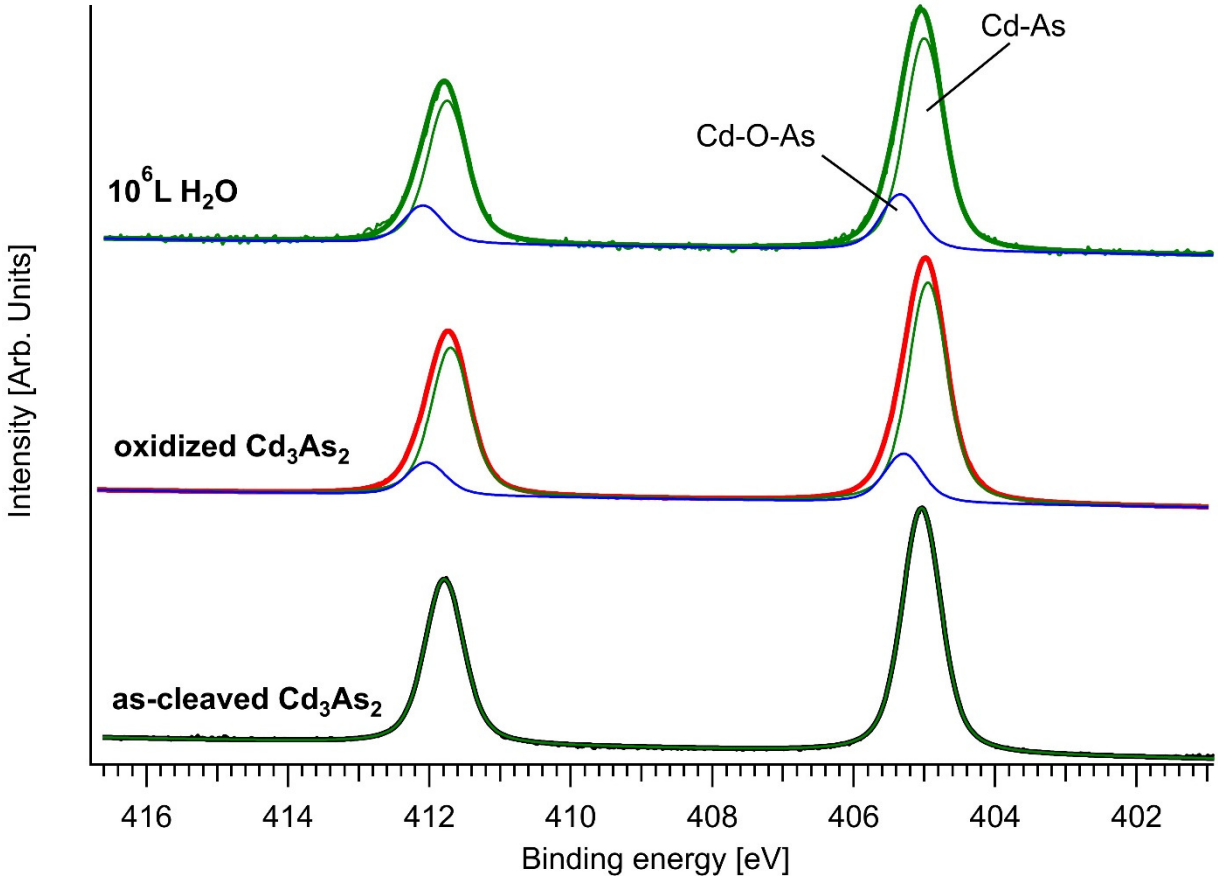

Figure S5. Cd-3d for as-cleaved Cd_3As_2 (black curve), oxidized Cd_3As_2 obtained by exposing the as-cleaved sample to $5 \cdot 10^4$ L of O_2 (red curve) and the same oxidized surface after exposure to 10^6 L (green curve) of H_2O at room temperature. The incident photon energy is 610 eV. After O_2 exposure the main Cd-As component is slightly down-shifted due to oxygen intercalation and a new doublet with J=5/2 at BE~405.3 eV ascribed to hybrid Cd-O-As bonds appears.

Figure S6. Low-energy electron diffraction (LEED) image of a freshly cleaved Cd_3As_2 crystal. The first-order diffraction spots are arranged in the pseudo-hexagonal symmetry characteristic of the (112) natural cleavage plane. Blue hexagons denote the surface Brillouin zone (SBZ). Taken from our previous publication on Ref. [1]. (Copyright American Physical Society, 2018)

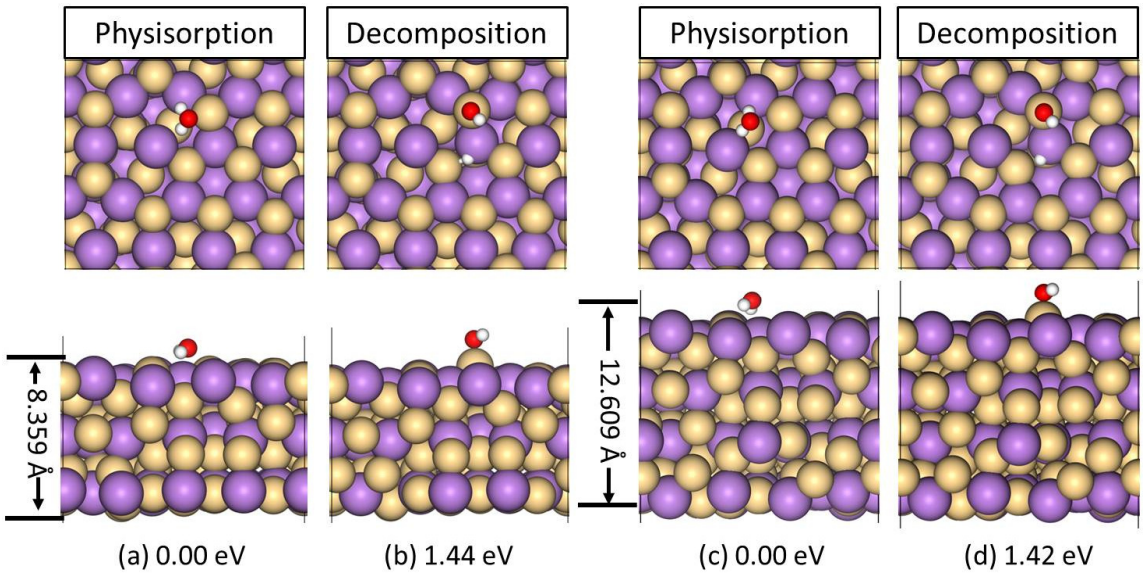

Figure S7. (a) Top and (c) side views of the adsorption configuration for H_2O adsorption at pristine $Cd_3As_2(112)$ surface with different thickness, respectively. Panels (b) and (d) show the H and OH fragments adsorbed at pristine $Cd_3As_2(112)$ surface with different thickness, respectively. Purple, brown, white and red balls denote As, Cd, H and O atoms, respectively.

1. S. Roth, H. Lee, A. Sterzi, M. Zacchigna, A. Politano, R. Sankar, F. Chou, G. Di Santo, L. Petaccia, O. Yazyev and A. Crepaldi, *Phys. Rev. B*, 2018, **97**, 165439.