SUPPORTING INFORMATION

Unveiling the Catalytic Potential of Topological Nodal-Line Semimetal

AuSn₄ for Hydrogen Evolution and CO₂ Reduction

Danil W. Boukhvalov^{1,2}, Gianluca D'Olimpio³, Federico Mazzola⁴, Chia-Nung Kuo⁵, Sougata Mardanya⁵, Jun Fujii⁴, Grazia Giuseppina Politano⁶, Chin Shan Lue⁵, Amit Agarwal⁷, Ivana Vobornik⁴, Piero Torelli⁴, Antonio Politano³

¹ College of Science, Institute of Materials Physics and Chemistry, Nanjing Forestry University, Nanjing 210037, P. R. China

² Institute of Physics and Technology, Ural Federal University, Mira Str. 19, 620002 Yekaterinburg, Russia

³ Department of Physical and Chemical Sciences, University of L'Aquila, via Vetoio, 67100 L'Aquila (AQ), Italy

⁴ 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

 ⁵ Department of Physics, National Cheng Kung University, 1 Ta-Hsueh Road, 70101 Tainan, Taiwan
⁶ Department of Information Engineering, Infrastructures and Sustainable Energy (DIIES), University "Mediterranea" of Reggio Calabria, Loc. Feo di Vito, 89122 Reggio Calabria, Italy
⁷ Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India.

S1. O-1s core level of AuSn₄ before and after exposure to O₂, CO, H₂O and air

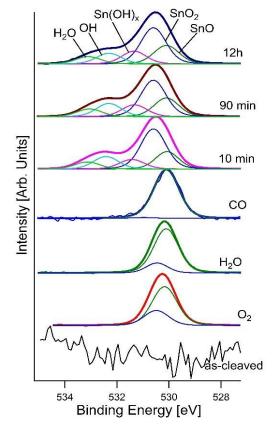


Figure S1: O-1s Core-level spectra collected from ascleaved AuSn₄ (black curve) and from the same surface exposed to O_2 (red curve), H_2O (green curve) and CO (blue curve). The AuSn₄ surface was also exposed to air for different times, 10 minutes (pink curve), 90 minutes (brown curve) and 12 hours (dark blue curve). The photon energy is 900 eV and the spectra are normalized to the maximum.

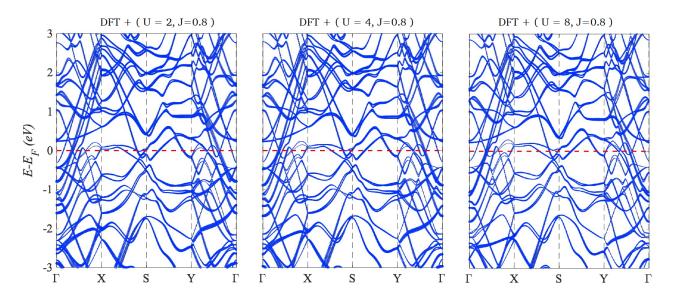


Figure S2: Band structure calculated with DFT+U, with U=2, 4, 8 eV