

Abstract Submitted  
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**Topological Insulators as Substrates for CO Oxidation Catalysis by Ultrathin Au Films**<sup>1</sup> HUA CHEN, U of Tennessee-Knoxville, WENGUANG ZHU, U of Tennessee-Knoxville; Oak Ridge National Laboratory, DI XIAO, Oak Ridge National Laboratory, ZHENYU ZHANG, Oak Ridge National Laboratory; U of Tennessee-Knoxville; ICQD/HFNL, USTC — We propose a novel application of three dimensional topological insulators (3DTIs) in heterogeneous catalysis based on first- principles calculations within density functional theory. We use a  $\text{Bi}_2\text{Se}_3$  substrate as the support of an ultrathin Au film, and show that the Au adatoms are strongly bound to and able to wet the surface of  $\text{Bi}_2\text{Se}_3$ . More importantly, we find the topological surface states of  $\text{Bi}_2\text{Se}_3$  are robust against Au deposition, and it can enhance the interaction between Au and CO,  $\text{O}_2$  molecules by acting as an “electron bath”. The present study may broaden the potential technological applications of 3DTIs, and shine some new light on the understanding of the role of surface states in heterogeneous catalysis.

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