

# False-positive and false-negative assignments of topological insulators in density functional theory and hybrids

J. Valenzuela,<sup>1</sup> X. Zhai,<sup>2</sup> L. Yang,<sup>1</sup> J.-W. Liu,<sup>1</sup> and A. Zunger<sup>1,\*</sup>

<sup>1</sup>National Renewable Energy Laboratory, Golden, Colorado 80401, USA

<sup>2</sup>Department of Physics, Colorado School of Mines, Golden, Colorado 80401, USA

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Density functional theory (DFT) and hybrid functionals are used to study the electronic structure of topological insulators (TIs) and semiconductors. We show that the band structure of TIs is highly sensitive to the choice of the exchange-correlation functional. In particular, we demonstrate that the band structure of TIs can be incorrectly assigned as that of a semiconductor or a metal when using standard DFT functionals. This is due to the fact that the band structure of TIs is highly sensitive to the choice of the exchange-correlation functional. In particular, we demonstrate that the band structure of TIs can be incorrectly assigned as that of a semiconductor or a metal when using standard DFT functionals. This is due to the fact that the band structure of TIs is highly sensitive to the choice of the exchange-correlation functional.

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Topological insulators (3D) and 2D topological insulators (TI) are a new class of materials that have attracted much attention in the past few years. The band structure of TIs is highly sensitive to the choice of the exchange-correlation functional. In particular, we demonstrate that the band structure of TIs can be incorrectly assigned as that of a semiconductor or a metal when using standard DFT functionals. This is due to the fact that the band structure of TIs is highly sensitive to the choice of the exchange-correlation functional.

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Methods. Calculations were performed using density functional theory (DFT) and hybrid functionals (HF). The band structure of TIs is highly sensitive to the choice of the exchange-correlation functional. In particular, we demonstrate that the band structure of TIs can be incorrectly assigned as that of a semiconductor or a metal when using standard DFT functionals. This is due to the fact that the band structure of TIs is highly sensitive to the choice of the exchange-correlation functional.

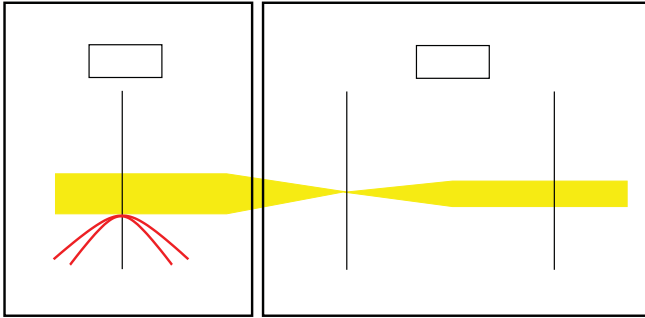


TABLE II. Calculated band structure of  $\text{C}_6\text{T}_7(\text{S}_2\text{S})_2$  using DFT (HSE06) and GW methods. The energy difference between the conduction band minimum and the valence band maximum is denoted by  $\Delta_i$ . The band structure is shown for the  $\Gamma$  point (left) and the  $\Gamma$  point (right).

Energy (eV)	$\Gamma$ point	$\Gamma$ point
10.0		
9.0		
8.0		
7.0		
6.0		
5.0		
4.0		
3.0		
2.0		
1.0		
0.0		
-1.0		
-2.0		
-3.0		
-4.0		
-5.0		
-6.0		
-7.0		
-8.0		
-9.0		
-10.0		

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