

Abstract Submitted  
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**Prediction of a “half semiconductor” for spintronics in non-compensated n-p codoped  $\text{TiO}_2$** <sup>1</sup> WENGUANG ZHU, University of Tennessee & Oak Ridge National Laboratory, XING-QIU CHEN, Institute of Metal Research, CAS, China, HANNO WEITERING, University of Tennessee & Oak Ridge National Laboratory, ZHENYU ZHANG, University of Science and Technology of China & Harvard University, G. M. STOCKS, Oak Ridge National Laboratory — Based on hybrid density functional calculations, we predict that by doping non-compensated Cr-N pairs a normal wide-band-gap semiconductor  $\text{TiO}_2$  can be altered to a “half semiconductor”, in which both the top and the valence band and the bottom of the conduction band are fully spin-polarized and exclusively contributed by the same spin component. The underlying formation mechanism of such an unusual band structure is revealed via detailed electronic structure analysis. The magnetic property of the material will also be discussed in this talk. Such a “half semiconductor” material may provide a new twist to generate and manipulate spin currents for spintronics.

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