Abstract Submitted
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Design of transparent conductors and periodic two-dimensional electron gases without doping XIUWEN ZHANG, LIJUN ZHANG, ALEX ZUNGER, Renewable and Sustainable Energy Institute, University of Colorado, Boulder, Colorado, JOHN PERKINS, National Renewable Energy Laboratory, Golden, Colorado, MATERIALS BY DESIGN TEAM, JOHN D. PERKINS COLLABORATION — The functionality of transparency plus conductivity plays an important role in renewable energy and information technologies, including applications such as solar cells, touch-screen sensors, and flat panel display. However, materials with such seemingly contraindicated properties are difficult to come by. The traditional strategy for designing bulk transparent conductors (TCs) starts from a wide-gap insulator and finds ways to make it conductive by extensive doping. We propose a different strategy [1] for TC design—starting with a metallic conductor and designing transparency by control of intrinsic interband transitions and intraband plasmonic frequency. We identified specific design principles for prototypical intrinsic TC classes and searched computationally for materials that satisfy them. The electron gases in the 3D intrinsic TCs demonstrate intriguing properties, such as periodic 2D electron gas regions with very high carrier density. We will discuss a more extended search of these functionalities, in parallel with stability and growability calculations. [1] X. Zhang, L. Zhang, J. D. Perkins, and A. Zunger, Phys. Rev. Lett. 115, 176602 (2015). Supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Grant No. DEFG02-13ER46959.

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