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GW-BSE calculations on two-dimensional MXene phases[1]
ZHENGLU LI, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory, LIANG HONG, Department of Physics, University of Illinois at Chicago, FELIPE JORNADA, TING CAO, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory, SERDAR OGUT, Department of Physics, University of Illinois at Chicago, STEVEN G. LOUIE, Department of Physics, University of California at Berkeley; Materials Sciences Divisions, Lawrence Berkeley National Laboratory — MXene is a promising candidate for new useful two-dimensional (2D) crystals. Experimentally, few-layer samples have been made from the bulk, and they demonstrate many excellent properties for electric and thermal transport, as well as other novel physics. In this work, we have performed GW-BSE calculations based on first-principles calculations to study some of the MXene family. We find that monolayer Ti_2CO_2 possesses insulating properties. Furthermore, the 2D screening effect is very strong, resulting in a GW band gap correction of almost 1 eV. Based on these initial results, we expect that optical properties of these materials will also have strong excitonic effects.

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Zhenglu Li
Department of Physics, University of California at Berkeley

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