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Nanosheets of MgB₂ as a new class of 2D semiconductor BO XU, SCOTT BECKMAN, Washington State Univ — The discovery of two-dimensional semiconducting materials, a decade ago, spawned an entire sub-field within solidstate physics that is focused on the development of nanoelectronics. Here we present a new class of semiconducting two-dimensional material based on hexagonal MgB₂. Although MgB₂ is a semimetal, similar to the other well-studied transition metal diborides, we demonstrate that, unlike the transition metal diborides, thinning MgB₂, to create nanosheets, opens a band gap in the density of states. We predict that a 7 Å thick MgB₂ nanosheet will have a band gap of 0.51 eV. MgB₂ nanosheets differ from other two-dimensional semiconductors in that the band gap is introduced by (001) surfaces and is opened by the quantum confinement effect. The implications of these findings are that nanostructured MgB₂ is not merely a new composition, but also has intrinsic mechanisms for tuning its electronic properties, which may facilitate the development of nanoelectronics.

> Bo Xu Washington State Univ

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