Van der Waals layered $MoSi_2N_4$ family

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Identifying 2D layered materials in the monolayer limit has led to discoveries of numerous new phenomena and unusual properties. We proposed a general concept to create new 2D layered materials without known 3D parents by passivating the dangling bonds of 2D nonlayered crystals with proper elements [1]. To this end, we first developed a novel CVD method with bilayer metal substrate to grow high-quality nonlayered 2D transition metal carbides/nitrides with diverse structures [2]. Interestingly, we found that introducing elemental silicon during CVD growth of 2D molybdenum nitride can passivate its surface dangling bonds, which enabled the growth of centimeter-scale monolayer films of a new van der Waals layered material, $MoSi_2N_4$ [2]. This monolayer material can be viewed as a MoN_2 sandwiched between two Si-N bilayers and exhibits semiconducting behavior (bandgap, ~1.94 eV) with a potentially high carrier mobility up to 1200 cm^2/Vs, high strength (~66 GPa), good thermal conductivity (~173 W/mK), and excellent ambient stability [1,3]. When multilayer MoN was sandwiched between the two Si-N bilayers, a 2D superconducting $MoSi_2N_4(MoN)_{4n}$ homologous compound was formed [4]. Density functional theory calculations further predicted a large family of $MoSi_2N_4$-structured 2D layered materials with a general formula MA_2Z_4 [1,5], including semiconductors, metals, magnetic half-metals, superconductors, and topological insulators, which are expected to have promising applications in electronics, spintronics, valleytronics, optoelectronics, energy conversion and storage, and thermal management.

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