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Stability and magnetism in FeC_2 monolayer TIANSHAN ZHAO, Peking University, JIAN ZHOU, Department of Physics, Virginia Commonwealth University, QIAN WANG, Center for Applied Physics and Technology, Peking University, YOSHIYUKI KAWAZOE, New Industry Creation Hatchery Center, Tohoku University, PURU JENA, Department of Physics, Virginia Commonwealth University — We report a new FeC_2 sheet containing C_2 dimers, which can be chemically exfoliated from bulk $ThFeC_2$ phase. Using density functional theory combined with AIMD and phonon dispersion calculation, we found that upon exfoliation from bulk $ThFeC_2$, the FeC_2 sheet changes its symmetry from *Amm*2 to *Pmmn*, while retaining its robust dynamical, thermal and mechanical stability. In sharp contrast to the metallic and paramagnetic bulk phase of $ThFeC_2$ and the recently reported TiC_2 sheet, the exfoliated FeC_2 sheet is half-metallic and ferromagnetic with a Curie-temperature of 245 K, making it a promising candidate for spintroinc applications.

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