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Search for giant magnetic anisotropy in transition-metal dimers on defected hexagonal boron nitride sheet[1] JIE LI, State Key Lab. of Surface Physics, Key Lab. of Computational Physical Sciences, and Dept. of Physics, Fudan Univ. , HUI WANG, Dept. of Physics and Astronomy, Univ. of California, JUN HU, College of Physics, Optoelectronics and Energy, Soochow Univ. , RUQIAN WU, Dept. of Physics and Astronomy, Univ. of California — For a magnetic units at the nanometer scale, one of the most important issues is how to hold thermal fluctuation of its magnetization, i.e., how to enhance its blocking temperature ($T_{\$\_B\$}$) to above 300K. Through systematic density functional calculations, the structural stability and magnetic properties of many transition-metal dimers embedded in a defected hexagonal boron nitride monolayer are investigated. We find twelve cases that may have magnetic anisotropy energies (MAEs) larger than 30 meV. In particular, Ir-Ir@Dh-BN has both large MAE (˜126 meV) and high structural stability, which makes it a promising candidate of magnetic unit in spintronics and quantum computing devices.

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