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**Half-Metallicity in Two-Dimensional Nickel Cyanide Molecular Layers** CRAIG HIGGINS, GARY BEALL, BYOUNGHAK LEE, Texas State University — We investigate the electronic structural properties of undoped- and doped-transition metal nickel cyanide molecular layers. Our theoretical study is motivated by recent experiments synthesizing two-dimensional nickel cyanides from a reaction of nickel tetracyanides and other divalent transition metals [1]. DFT calculations reveal that, while the undoped molecular planar structure is a narrow band gap semiconductor with a band gap of 0.3 eV, the structures with iron doping are half-metals. We discuss the stability of the ferromagnetic phase and the effective magnetic coupling between magnetic ions. We confirm the calculated results by comparing with atomic force microscopy and tunneling electron microscopy measurement.

[1] G. Beall, private communication

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