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NiMoO₃, a new half metal predicted by first principles¹ ZHIJIAN WU, JING WANG, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences — Half-metallic (HM) materials are metallic for one spin direction while at the same time semiconducting for the other spin direction [1]. In our recent study, NiMoO₃ is designed and studied by the first principles [2]. It is isostructural and isovalent to experimental synthesized NiCrO₃. Compensated half metal is obtained when considering electron correlation alone. Inclusion both spin - orbit coupling and electron correlation induce a large orbital moment on Ni (- 0.23 μ B) due to the Coulomb enhanced spin - orbit coupling. This makes NiMoO₃ a half metallic ferrimagnet with nonintegral magnetic moment.

[1] de Groot, R. A.; Mueller, F. M.; van Engen, P. G.; Buschow, K. H. J. Phys. Rev. Lett., 1983, 50, 2024.

[2] Wang, J., Wu, Z. J. Appl. Phys. Lett, 2012, 101, 042414.

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