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 µB) due to the Coulomb enhanced spin - orbit coupling. This makes NiMoO₃ a half metallic ferrimagnet with nonintegral magnetic moment.

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