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**Computational study of novel half metallic compounds** ZHIJIAN

WU, JING WANG, Changchun Institute of Applied Chemistry — Half-metallic (HM) materials are metallic for one spin direction while at the same time semi-conducting for the other spin direction [1]. The unique feature of HM material is that it has an integer spin magnetic moment. For a carefully selected material, the integer can be zero (compensated). Besides ferromagnetic (FM) parallel spin arrangements, ferrimagnetic or even antiferromagnetic (AFM) alignments are also possible. In particular, half-metallic antiferromagnet (HM-AFM) possesses no macroscopic magnetization, yet their carriers are fully spin-polarized. In this work, half metallic compounds have been predicted by using the first principles, such as NiMoO<sub>3</sub> [2].

[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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