

V_nBz_{n+1} . In these V_nBz_{n+1} system, V ions are arranged in ferromagnetic state. Meaningfully, our results reveal an interesting nonmonotonous magnetic behavior caused by finite-size effect, and the energy cost for reversing the magnetic moment of the edge V oscillates with n . $V(Bz)_\infty$ is a proper material for spin-polarized transport and has high stability in the presence of electronic and magnetic field.

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- [1] L.P. Zhou, S.W. Yang, M.F. Ng, M.B. Sullivan, V.B.C. Tan and L. Shen, J. AM. Chem. Soc. **130**, 4023 (2008)
 - [2] L. Shen, S.W. Yang, M.F. Ng, V. Ligatchev, L.P. Zhou and Y.P. Feng, J. AM. Chem. Soc. **130**, 13956 (2008)
 - [3] L. Wang, Z.X. Cai, J.Y. Wang, J. Lu, G.F. Luo, L. Lai, J. Zhou, R. Qin, Z.X. Gao, D.P. Yu, G.P. Li, W.N. Mei, and S. Sanvito, Nano Letters **8**, 3640 (2008)
 - [4] K. Miyajima, A. Nakajima, S. Yabushita, M.B. Knickelbein and K. kaya, J. AM. Chem. Soc. **126**, 13202 (2004)
 - [5] J.T. Lyon and L. Andrews, J. Phys. Chem. A **109**, 431 (2005)
 - [6] K. Miyajima, S. Yabushita, M.B. Knickelbein and A. Nakajima, J. AM. Chem. Soc. **129**, 8473 (2007)
 - [7] J.L. Wang, P.H. Acioli and J. Jellinek, J. AM. Chem. Soc. **127**, 2812 (2005)
 - [8] H. Weng, T. Ozaki and K. Terakura, Phys. Rev.B **79**, 235118 (2009).
 - [9] X.J. Wu and X.C. Zeng, J. AM. Chem. Soc. **131**, 14246 (2009)
 - [10] V.V. Maslyuk, A. Bagrets, V. Meded, A. Arnold, F. Ever, M. Brandbyge, T. Bredow and I. Mertig, Phys. Rev. Lett.**97**, 097201 (2006).