

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Unusual Structure and Magnetism in MnO Nanoclusters¹ SHREE-MOYEE GANGULY, Ph.D. student, S. N. Bose National Center for Basic Sciences, Kolkata, India, MUKUL KABIR, Postdoctoral researcher, MIT, USA, BIPLAB SANYAL, Associate Professor, Uppsala University, Sweden, ABHIJIT MOOKERJEE, Professor, S. N. Bose National Center for Basic Sciences, Kolkata, India — We report an unusual structural and magnetic evolution in stoichiometric MnO nanoclusters by an extensive and unbiased search through the potential energy surface within density functional theory. The $(MnO)_n$ nanoclusters adopt two-dimensional structures in size ranges in which Mn_n nanoclusters are three-dimensional and regardless of the size of the nanocluster, the magnetic coupling is found to be antiferromagnetic, and is strikingly different from Mn-based molecular magnets. Both of these features are explained through the inherent electronic structures of the nanoclusters.

¹We gratefully acknowledge financial support from Swedish Research Links program funded by VR/SIDA and Carl Tryggers Foundation, Sweden.

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Date submitted: 19 Nov 2010

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