Skoltech
Skolkovo Institute of Science and Technology

When: Wendsday, Sep 11, at 12:00-13:00
Where: Blue Bldg (TPOC-3), room 408

COMPUTATIONAL MATERIALS SCIENCE SEMINAR

BOOSTING ANALYTICAL PROPERTIES OF PLASMONIC SPIKED PARTICLES

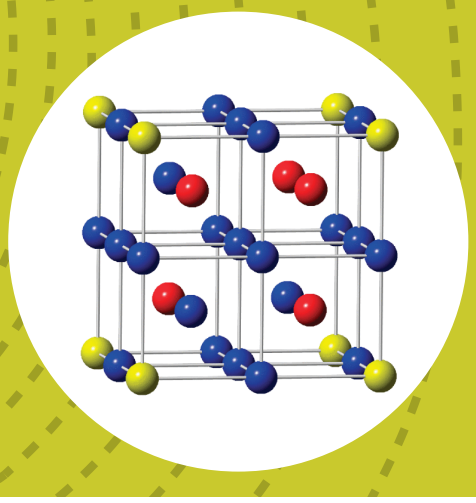

Fig. 1. Atoms are Co (blue), Mn (red), and Fe (yellow).

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ABSTRACT

The talk aims at presenting our research investigations on high-moment magnetic alloys based on Manganese. The main thrust of the research is on pinpointing the atomic positions and their effect on the net magnetization in Mn-based and Mn-doped alloys. These systems are of great interest because of their potential to provide a whole range of magnetization based on the exchange interactions in the system. Isolated manganese atoms have half-filled 3d shells and a magnetic moment of 5 μ B , which would correspond to a magnetization M s (polarization μ o M s) of approximately 5 T in dense-packed Mn magnets. If this magnetization could be realized in ferromagnetic materials, it would revolutionize technology, in particular since Mn is a relatively inexpensive element. However, known Mn-based permanent magnets, such as MnAl, MnBi, and Mn_2Ga, exhibit rather a modest magnetizations [1]. The main reason is the relatively low net magnetic moment, of the order of 0.5 μ B per atom, which means that 99% of the energy product is wasted. Itinerant-electron effects somewhat reduce the Mn moment [1], but the main reason for the low magnetization of most Mn alloys is the element's tendency to form antiferromagnetic interatomic exchange bonds. This feature has its origin in the nearly half-filled 3d shell, which destabilizes the ferromagnetic states through the forced occupancy of antibonding states [2]. In our earlier work [3], we provided a possible explanation for the experimentally observed high magnetizations in a range of bcc-type Fe-Co-Mn thin films deposited on MgO by Snow et al. [4]. We used density-functional calculations [3] to explain the high Fe-Co-Mn net magnetic moment. Our DFT and model calculations suggests that nature can be “tricked” into creating ferromagnetic order in Mn-rich alloys. Here, we will present a data mining approach to see the pattern and evaluate the correlation of the Mn-neighborhood with the magnetism in Mn-based alloys.

[1]. J. M. D. Coey, J. Phys. Condens. Matter 26, 064211-1-6, 2014.
[2]. R. Skomski and J. M. D. Coey, Institute of Physics, Bristol 1999.
[3]. A. Kashyap, R. Pathak, D. J. Sellmyer, and R. Skomski, IEEE Trans. on Magn., 54, 11, 2018.

BIOGRAPHY

Dr Arti Kashyap works as Associate Professor at IIT Mandi. She holds joint appointment in School of Basics Sciences and School of Computer and Electrical Engineering. She is awarded the prestigious Simon’s Associate from ICTP, Italy in 2015. Her main research interests are in electronic structure calculations using first principles approach and study of properties of magnetic nano-materials. Further, she has widened her research interests to databases and big data technologies/distributed computing. She is also very passionate to serve the society, particularly through educational activities and technological intervention. She has established “UHL Center” at IIT Mandi where the activities of social outreach are pursued with the funding from various Govt agencies, mainly, DST, Govt of India. She has many collaborations and the most recent one with the group of A. Popov at Ekterineburg under Indo-Russian funding.

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LOOKING FORWARD TO SEEING YOU!