Abstract Submitted
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Electronic structure theory of wide gap dilute magnetic semiconductors[1] LINHUI YE, A.J. FREEMAN, Northwestern University — The recent exciting reports that wide gap semiconductors, most notably ZnO, TiO_2 and GaN, when doped with transition metal elements, may have Tc's that are higher than room temperature have attracted great interest. When interpreted with care, highly precise first principles FLAPW calculations such as used here[2], are now providing insights into the nature of their strong ferromagnetism (FM). Here, we present an analysis to the electronic structures of several typical wide gap DMS's and illustrate how first principles calculations can lead to correct predictions of their magnetic properties for both Cr:TiO_2 and Mn:GaN. The results demonstrate the importance of defect compensation in the determination of the magnetism. A comparison between Mn:ZnO and Co:ZnO highlights the fundamental difference in their electronic structures which explains why their FM is dependent on carriers of different polarity. Correct predictions of their magnetism are found to be due to the correct treatment of the LDA band gap problem. Finally, we provide semi-quantitative discussions of Co doped TiO_2, and illustrate why it is highly non- trivial to fully explain its FM based on first principles calculations.

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[2]E.Wimmer,H.Krakauer,M.Weinert,A.J.Freeman, PRB **24**, 864(1981)

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