Condensed Matter / Quantum Information Seminar

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BROIDA ROOM 3302

INTERFACES IN CO-DOPED TIO2 ANATASE - THE KEY TO UNDERSTANDING THIS NEW CLASS OF DILUTED MAGNETIC SEMICONDUCTORS?

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About three years ago Co-doped TiO2 anatase was discovered to exhibit ferromagnetism at and above room temperature, i.e. to be a magnetically robust diluted magnetic semiconductor (DMS). Since then it has attracted considerable interest within the spintronics community, and a large amount of data can be found in the literature. However, there is still controversy over the origin of the magnetism as well as the influencing factors. So far it is believed that oxygen vacancies promote magnetism in Co-doped TiO2, and there is evidence that interfaces play a crucial role in determining the magnitude of the observed magnetic moments in these systems. In our work we address these two features in a systematic study by means of ab-initio density-functional calculations employing norm-conserving pseudopotentials and plane waves.
In our ongoing work we investigate the magnetic properties of bulk TiO2 anatase with substitutional Co-dopants and oxygen vacancies at various sites. Furthermore, starting with the low-energy Sigma-5(113)[-110] grain boundary in anatase, we study the relationship between microstructure and macroscopic magnetic properties. In this talk I will start with a brief introduction into the field of diluted magnetic semiconductors, followed by an overview over the literature in the area of the oxide-based DMS, especially concerning Co-doped TiO2. Against this background I will present our own newest results, discussing whether there really is a relationship between the microstructure of the films and the magnetic properties and what is the origin of the ferromagnetism / the nature of the magnetic coupling in Co-doped TiO2.