



# Fe vacancies in FeO

A talk by Silvia Gallego

Instituto de Ciencia de Materiales de Madrid, Spain

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Among the magnetic transition metal oxides (MTO), FeO is singular in its high content of Fe vacancies. Their existence adds difficulties in the comparison of the measured properties of FeO to the rest of the MTO, and eases the transformation of FeO to magnetite. Surprisingly, the existence of Fe vacancies had not been considered within an ab initio framework until recently. Here we will present our ab initio results on bulk FeO with a realistic concentration of vacancies. We will show how defects tend to form clusters that modify the electronic and magnetic properties of FeO, introducing features that resemble those of magnetite. We will also show how the tetrahedral environment linked to Fe defects in the bulk is also important in the stabilization of the O-termination at (111) surfaces. Furthermore, it accounts for the puzzling high magnetization measured at reconstructed surfaces, and seems to play an active role in the stabilization of stoichiometric FeO films in the ultrathin limit.