Virtual BSC RS: Determining the magnetic order of Con+ (n ? 5) clusters by using multi-configurational calculations

Objectives

Abstract: The magnetism of transition metal clusters have been for decades a complicated puzzle, with experimental results disagreeing with calculations performed within the density functional theory formalism. In this talk, I will provide a key to this puzzle by investigating the lowest-energy spin states of cobalt cluster, Con+ (n ? 5), using advanced CASSCF/NEVPT2 calculations with very large active spaces. These very computationally demanding calculations are able to correctly predict the measured spin states of the clusters, in contrast to the widely used density functional theory, with results that depend on the selected exchange-correlation functional. The reasons for the failure of density functional theory, in opposition to CASSCF/NEVPT2, will be discussed, providing a solid framework for investigating other transition metal and transition metal oxide clusters.

Short bio: Piero Ferrari received his

M.Sc. degree in physics at the Pontifical Catholic University of Chile in 2013. In 2017, he obtained his Ph.D. degree at KU Leuven, Belgium. Since 2017, he works as a postdoctoral researcher, grant awarded by the Research Foundation ? Flanders (FWO).

Speakers

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