Ph.D. Course in Materials Science and Nanotechnology

University of Milano-Bicocca, Department of Materials Science, via Cozzi 55, 20125 Milano

March 8, 2019 – 11.00 a.m.

Seminar room - Department of Materials Science U5

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Recent development in the non-collinear spin density functional approach

We have developed a first-principles electronic structure calculation method. This employs the spin density functional theory and allows us to treat non-collinear magnetic structures and/or fully-relativistic (including spin-orbit interaction) effects. This level of approximation keeps a non-empirical approach and thus, may sometimes be called first-principles. We had applied these approaches to small magnetic clusters and the liquid oxygen. To my knowledge the latter work is still only one application of first-principles molecular dynamics simulation with non-collinear magnetic structure for disordered atomic structure [1]. In this decade, developments of the approach have been devoted to the introduction of spin-orbit interaction, the application of external electric field to slab systems. Such development may contribute to spin electronics (spintronics) applications [2,3]. Recently, our laboratory has implemented the van der Waals density functional approach within our conventional computational code [4]. This approach successfully includes the dispersion force acting on molecules in a non-empirical way and enables us to access to a much wide range of target systems.

In the presentation, I will introduce some recent developments and applications in the non-collinear spin approach and applications [5], and discuss perspectives.

[1] T. Oda and A. Pasquarello, Phys. Rev. Lett. 89, 197204 (2002).

[2] M. Tsujikawa, S. Haraguchi, and T. Oda, J. Appl. Phys., 111, 083910 (2012).

[3] K. Sakamoto et al., Nat. Commun. 4, 2073 (2013).

[4] M. Obata et al., J. Phys. Soc. Jpn. 82, 093701 (2013); 84, 024715 (2015).

[5] M. Obata, M. Christivana, and T. Oda, AIP Advances 8, 101419 (2018).

PhD students and all interested in the seminar are kindly invited to participate.

The PhD Coordinator

Prof. Marco Bernasconi