Condensed Matter Physics Seminar

February 24th, Wednesday 15：00-16：00
Seminar room,
Theoretical Research Building, Namiki

First principles calculations in magnetic and disordered compounds

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The understanding and 'in-silico' optimization of magnetic compounds, in terms of composition and/or taking partially into account also temperature effects, benefits from various theoretical developments and methodological advancements of different types. One aspect of importance relates to the possible loss of long-range order, or ideal periodicity in the sample: doping or alloying can be a route for applied material science improvements, but have also offered a successful conceptual framework for describing the paramagnetic phase of some magnetic compounds.

In these situations application of density functional theory becomes more complicated, and reproducing physical results requires a good handling also of the disorder aspects. Sharing roots with dynamic field theory, the coherent potential approximation has historically provided the right tool to overcome difficulties. I will briefly report on the subject, addressing in particular work towards overcoming initial limitations of the prescription, and possible insight across different levels of application.

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