RCMS ·IGER Seminar

"Approaching multifunctionallity through computational simulations of magnetic and photo-sensiblemolecular materials"

Lecturer : Dr. Alex Domingo
(University of Strasbourg)

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Approaching multifunctionallity through computational simulations of magnetic and photo-sensible molecular materials

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Abstract

The design and synthesis of multifunctional materials with both electronic and magnetic properties is a big challenge that demands the best of our predicting capabilities. Combining these two complementary properties requires a detailed understanding of them individually. State-of-the-art computational techniques based on wave function methods can offer new insights about the underlying physics controlling the magnetism and electron transport of molecular materials. A couple of examples are the ferromagnetism of materials based on organic biradicals, and the photo-induced processes found on bimetallic compounds. Ultimately, the goal is to relate the structural factors that will allow us to control these phenomena and design new materials knowing their macroscopic properties in advance.