



21st October 2015 - 2:00 p.m.
CFEL-bldg. 99, seminar room IV

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Chemical control of spin coupling in molecules - a theoretical analysis

The control of spin states in molecules is crucial not only for a variety of potential applications such as molecular memory elements or switches, but also interesting from a fundamental science point of view. This control can be achieved, e.g., by manipulating the chemical composition of spin centers and bridging ligands, by varying temperature, pressure or external fields, or by mechanical means. We discuss examples for how theory can help in achieving spin state control, and which challenges this poses for present-day theoretical methodology, in particular for Kohn-Sham density functional theory.