Universität Bielefeld Fakultät für Physik

Condensed Matter Theory Seminar

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DFT From A-Z with Emphasis on MM

In this presentation I will talk about the basics of density-functional theory (DFT) for performing calculations on molecules and clusters. I will include an overview on how to perform such calculations, why DFT is a popular framework for quantum science, and what properties are appropriate for simulation within DFT. Practical examples, concentrating on vibrations, electronic structure, and magnetism will be briefly surveyed. As an example of recent uses for the study of molecular magnets, I will give an overview of new calculations that predict the presence of low-energy spin-flip excitons in the Mn12-Acetate molecules [1].

[1] Electronic and Magnetic Signatures of Low-Lying Spin-Flip Excitonic States of Mn12O12-Acetate, Karma Dema, Zahra Hooshmand, and Mark R. Pederson (Submitted to polyhedron).

Thursday, 20.05.2021, 16:00 CEST
online/zoom