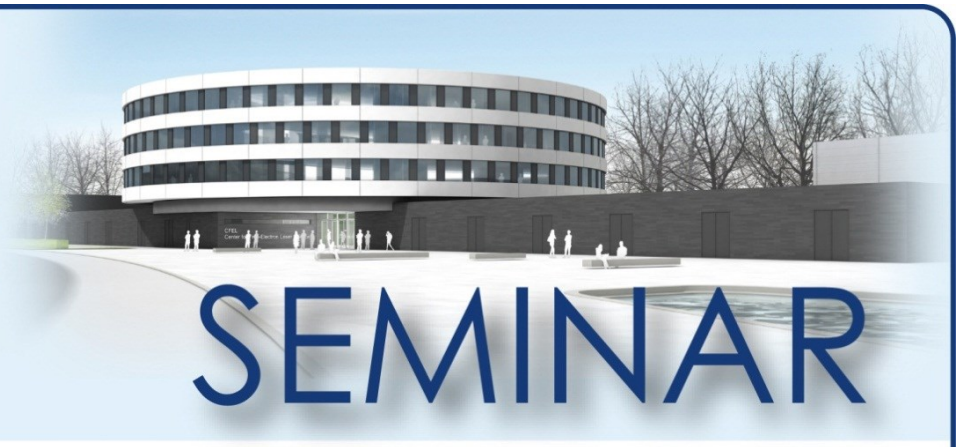
CFEL SCIENCE



SEMINAR

8th November 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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Fully non-local approximations for density functional theory

Density Functional Theory (DFT), a formalism that makes quantum mechanical calculations doable in a reasonable time, is the fundamental building block of the successes of computational chemistry and materials science in understanding and guiding experiments. DFT is able to capture the quantum nature of electrons, but relies on approximations to describe the interactions between them. The exact mathematical form of these interactions within DFT is not known, and people have to make educated guesses, possibly fitting experimental data. These approximations are successful in many cases, but typically fail when electronic interactions play a prominent role (strong correlation). I will illustrate an approach to the problem from a different perspective, by looking at the limit in which the interaction between the electrons becomes infinitely strong, which we have studied carefully in the recent years. Despite how bizarre this limit might sound, it has the advantage of unveiling the mathematical DFT structure of the electronic interactions. I will review rigorous results for this limit, including its higher-order corrections, and discuss new approximations inspired to them.

Host: Robin Santra – CFEL-DESY Theory Division