hyperfine properties of solids calculated from first principles: why do we care?

Experimentally determined hyperfine parameters in solids are a useful tool to unravel problems in fundamental as well as applied condensed matter physics. Nowadays, hyperfine properties can be routinely computed from first principles as well. In this seminar, we will discuss the major computational tools that can be used for this purpose, with their strengths and limitations. Ample illustrations from the literature on magnetic hyperfine fields, electric-field gradients (quadrupole interaction) and isomer shifts will show how the combination of experiment and calculations in hyperfine research can lead to better insight, and sometimes even to new questions. At the end, we will zoom in on a 'new' hyperfine property that requires the highest possible experimental and computational accuracy to be detected: the quadrupole shift (analogous to the more familiar isomer shift, but for the quadrupole interaction).

The target audience for this seminar should have a general knowledge in physics/chemistry, but no previous knowledge on either hyperfine interactions or first principles calculations will be assumed.

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