First Principles Calculations for Materials with Strong Electronic Coulomb Correlations – Where Do We Stand?

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Engineering novel materials with predefined properties is the dream of computational materials scientists. Systems with strong electronic Coulomb interactions are particularly prone to a high tunability of relevant properties. Designing computational tools to deal with correlated electron systems in a materials-specific manner is thus a key step for pushing forward nowadays predictive capabilities.

In this talk, we review current strategies of combining dynamical mean field techniques with electronic structure theory, with illustrations on d- and f-electron systems. In the second part, we will discuss current open questions and challenges, and describe further perspectives on the way to truly predictive many-body theories.

Einführung: Prof. Dr. I. Eremin

Die Fakultät lädt alle Interessierten herzlich ein.

Ab 11.45 Uhr Kaffee/Tee im Hörsaal