

May 10, 2021 10:00 AM

QED & Materials seminar

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Title

“Electronic structure of correlated materials: new methods and applications”

Abstract

Strongly correlated materials show some of the most fascinating physical phenomena, but are at the same time very challenging to study theoretically.

In this talk, I will highlight recent results on cerium-based permanent magnets and new inorganic pigment materials. I will show how one can tackle the Kondo effect in the Ce-4*f* shell to calculate the magnetic anisotropy in permanent magnets and how the optical gaps and conductivities in the rare-earth fluorosulfides, novel correlated pigment materials, can be determined from first principles. Eventually, I will compare the theoretical results obtained from combined density functional theory and dynamical mean-field theory (DMFT) to experiment.