

MAR10-2010-020328

Abstract for an Invited Paper
for the MAR10 Meeting of
the American Physical Society

Materials Design using Correlated Materials – Where do we stand?

SILKE BIERMANN, CPHT, Ecole Polytechnique

Theory providing guidance for the fabrication of new materials or devices with given electronic properties, such is the dream of modern electronic structure theory. Where do we stand, and what are the possibilities and limitations nowadays? In this talk, we will discuss some examples of materials where strong electronic Coulomb interactions invalidate a simple band picture. We will review electronic structure techniques based on dynamical mean field theory, designed to cure such shortcomings. Results on transition metal oxides and pnictides will be used for illustration.