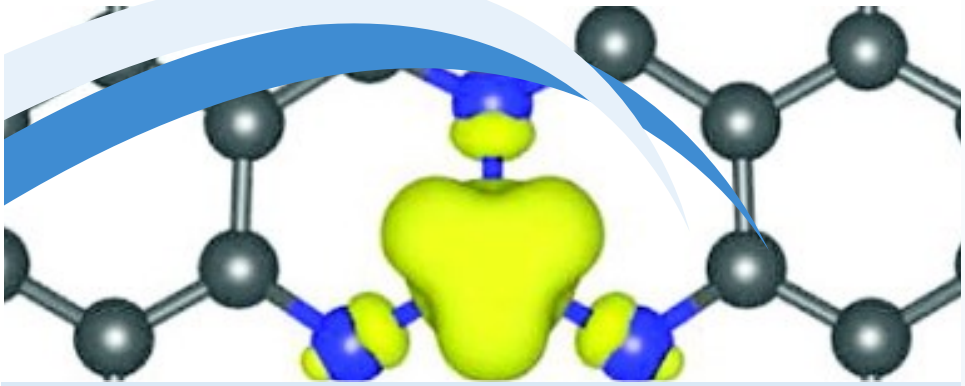
University of South Alabama Physics Department Colloquium

4:00 – 5:00 pm
Thursday, October 23, 2014
ILB Room 250

Refreshments are served starting at 3:45 pm



The Role of Quantum Mechanics in the Process of Materials Design

The laws of quantum mechanics form the basis for our understanding of the elements in the periodic table and their interactions in compounds. Materials science in the 20th century can be broadly characterized as evaluating the properties of particular materials in terms of these fundamental laws. With our increasing understanding of structure/property relationships the focus of materials science continues to shift toward rational materials design. However, while the fundamental physical laws of electrons in materials are well established, the a priori identification of candidate materials with particular targeted properties remains a significant challenge. I will discuss how our current understanding of the periodic table can inform our search of promising material sets for particular applications. Advanced computational methodologies are an integral part of this effort: They allow the evaluation of the effects of composition and crystal structure on electronic and magnetic properties before materials synthesis and provide invaluable guidance for materials selection. During the presentation I will address how our first-principle computations inform the design of novel 3d and 5d transition metal compounds with applications in spintronics and related areas.

Dr. Boris Kiefer

Associate Professor
Department of Physics
New Mexico State University

Dr. Kiefer's research specializes in computational material science. His research uses state-of-the-art simulation techniques to explore and predict material properties under a wide range of thermodynamic conditions.

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