

Physics Colloquium

UNIVERSITY OF MISSOURI-KANSAS CITY
DEPARTMENT OF PHYSICS

Professor Kazuyoshi Ogasawara

Department of Chemistry,
Kwansei Gakuin University,
JAPAN

First-principles calculations of $4f^n \rightarrow 4f^{n-1}5d$ transition spectra of rare-earth ions in crystals

Due to the growing demand for the lasers and phosphors operating in UV and VUV regions, a great deal of attention is being paid now to the thorough analysis of high lying energy levels of rare-earth (RE) ions arising from their $4f^{n-1}5d$ electron configurations. Although nonempirical prediction of optical spectra is quite important for development of novel optical materials, most conventional electronic structure calculation programs are not necessarily suitable for calculations of multiplet spectra. In order to overcome such a situation, we have developed a first-principles relativistic configuration-interaction (CI) calculation program, which is especially designed to calculate the multiplet spectra of metal ions in crystals. In this talk, a brief explanation of our first-principles relativistic CI program and its applications to $4f^n \rightarrow 4f^{n-1}5d$ transition spectra of RE ions in crystals will be presented.

Physics Department
Robert H. Flarsheim Science & Technology Hall
5110 Rockhill Road
University of Missouri-Kansas City

September 7, 2007

Coffee at 3:10, Colloquium at 3:30 in Room 310