

**Institute for Advanced Simulation  
Jülich Supercomputing Centre**

## **IAS Seminar**

**Topic:**           **Numerical analysis of augmented plane waves methods**

**Speaker:**       Prof. Dr. Reinhold Schneider, Institut für Mathematik, TU Berlin

**Contents:**       We analyze the augmented plane wave methods which are widely used in full-potential electronic structure calculations. We introduce a nonconforming method and the augmented methods are viewed as a special case. A priori error estimate is given and numerical experiments are presented to support our theory. Parts of the results are extended to Numerical Atomic Orbital basis functions.

**Time:**           Thursday, 26 April 2012, 15:15

**Venue:**           Jülich Supercomputing Centre, Hörsaal, building 16.3, room 006

Anyone interested is cordially invited to participate in this seminar.

sgd Prof. Dr. Stefan Blügel