New Perspectives in Efficient Large-Scale Modeling

Volker Eyert
Center for Electronic Correlations and Magnetism
Institute for Physics, University of Augsburg
86135 Augsburg, Germany
email: eyert@physik.uni-augsburg.de, volker@eyert.de

The ab initio calculation of materials properties has become an increasingly important task of modern materials science. In turn, the importance of materials science for the solution of some of mankinds most urgent problems, especially the environment-friendly and sustainable use of energy, is no longer a matter of dispute. This includes studies on materials to be used particularly in photovoltaics, water splitting, thermoelectrics, battery systems, and the like. For this reason, the development of computational methods for the efficient and accurate evaluation of materials properties on a large scale is highly desired. In this talk, I will report on recent developments and breakthroughs in the field. In particular, I will present ideas on efficient localized basis set ab initio methods, which combine the chemical intuiton and efficiency provided by such basis sets with new theoretical tools leading to a tremendous increase of accuracy, and which thus pave the way for efficient large-scale studies. Recent success of these developments is illustrated with examples and new results.