Title:

Parallelization and Optimization of the FLEUR Code: New Possibilities for All-electron Density Functional Theory

Author: **Uliana Alekseeva -** Forschungszentrum Jülich GmbH - Jülich - Germany

Abstract:

FLEUR (Full-potential Linearized augmented plane wave in EURope) is a code family for calculating ground-state as well as excited-state properties of solids within the context of density functional theory (DFT). A key difference with respect to the other MAX-codes lies in the treatment of all electrons on the same footing. Thereby we can also calculate the core states and investigate effects in which these states change. In this talk we show how performance optimizations and automation enhancements of the code allow for simulations of extremely big systems or automatically perform and analyze high-throughput calculations.