On behalf of the

Science College CMS

Vienna Computational Materials Laboratory

and Center for Computational Materials Science

we cordially invite you to the following seminar

Dipl.-Ing. Philipp Wissgott

Institute of Applied Physics, Vienna University of Technology, Austria

Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions

We present wien2wannier, an interface between the full-potential linearized augmented plane wave package Wien2k and the wannier90 code for the construction of maximally localized Wannier functions. The workflow starting from wien2k is shown step by step, including possible usages of the Wannier orbitals obtained from wannier90. Describing the main features of the algorithm, we introduce, as a simple example, the case of $SrVO_3$. We consider also a more elaborate example, $FeSb_2$, which is a compound with interesting thermoelectric properties. For this low symmetric material, we illustrate the procedure of obtaining a locally diagonal Wannier basis set from a wien2k bandstructure. These real space orbitals provide a convenient basis for DMFT calculations. We will be thus able to shine light on the effect of electronic correlations in compounds with a mixed d- and p-manifold at the Fermi edge.

J. Kuneš, R. Arita, P. Wissgott, A.Toschi, H. Ikeda, K. Held Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions, Comp. Phys. Commun. **181**, 1888(2010).

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Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10