



EINLADUNG zum IFP-SEMINAR

- Thema: **First-principles Study of Martensitic Phase Transformation of Ti-based Alloys**
- Vortragender: **Liang Si**
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- Host: Karsten Held
- Termin: **Mittwoch, 27 Februar 2013, 16 Uhr**
- Ort: Institut für Festkörperphysik, TU Wien
Wiedner Hauptstraße 8-10, 1040 Wien
Seminarraum 138C, 9. OG (gelbe Leitfarbe)
- Förderer: ERC-StG-306447 AbinitioDGA

It is well known that the shape memory effect is related to the martensitic phase transformation, which can occur for TiM (M belongs to the subgroup VIII in the periodic table, i.e. Ni, Rh, Ir, Pd, Pt) alloys on cooling. However, ground state structures of $TiRh$ and $TiIr$ are not clear yet. The phase transition process from high-temperature phase to low-temperature phase is still not clear in atomic level. We found out ground state structure and transformation path by study of eigenvibration directions corresponding to the softening frequencies mode in phonon dispersion spectrum. Meanwhile, the origin of such transition behaviors on cooling has not been discovered so far. The electronic configurations considering the d -orbital energy-level splitting of M atom in the crystal field and the phonon softening were studied. We found that the Jahn-Teller effect is responsible for martensitic phase transition.

