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. Evgeniya Kabliman

Institute of Materials Chemistry, Vienna University of Technology, Austria

Ab initio study of stabilization of the misfit layer compound $(PbS)_{1.14}TaS_2$

In the present work we perform *ab initio* electronic-structure calculations of the $(PbS)_{1.14}TaS_2$ misfit layer compound in order to understand the basic mechanism of its stabilization. Density-functional based calculations were carried out in commensurate unit cells containing 74 or 296 atoms using the WIEN2K code. The two experimentally predicted mechanisms of stabilization, namely, metal cross substitution (interchange of Pb and Ta atoms in the PbS and TaS_2 layers) and nonstoichiometry (substitution of Pb by Ta), were investigated. The results show clearly that the nonstoichiometry mechanism plays the significant role. When Pb inside the PbS layer is substituted by Ta with concentrations around 0.13–0.19, a stabilization is found with respect to the parent PbS and TaS_2 compounds. These results are explained by an analysis of partial densities of states. The calculated x-ray photoemission spectroscopy core-level shifts are in reasonable agreement with experiments.

Date: Monday, Oct 18, 2010 16:00

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