

COE セミナー

題目 : Combination of the KKR-method and the LSDA+DMFT scheme

日時 : 平成 18 年 9 月 22 日 (金) 16:40~

場所 : 理学部 H 棟中セミナー室 (H601)

講師 : Hubert Ebert 教授 (ミュンヘン大学, ドイツ)

要旨 :

The main features of the KKR-band structure are briefly reviewed including its spin-polarized relativistic version. Application to the valence band photoemission of noble metals demonstrates that a very good agreement can be achieved on this basis. This also applies for the spin-orbit induced Fano-effect. For the pure ferromagnets Fe, Co and Ni, however, discrepancies occur that have to be ascribed to correlation effects. To deal with this problem a combination of the KKR-method with the recently developed LSDA+DMFT (dynamical mean field theory) scheme was worked out. This combined KKR-DMFT approach leads to rather satisfying agreement, as it is demonstrated for ground state as well as spectroscopic properties.

連絡先 赤井久純 (Tel : 5738)