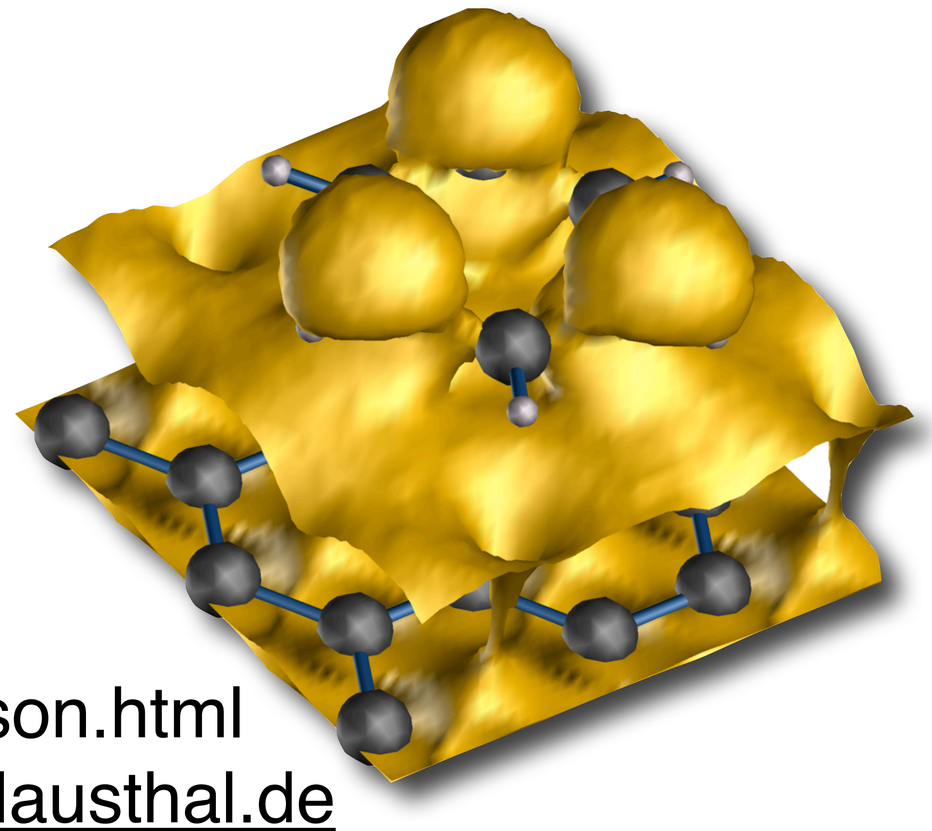
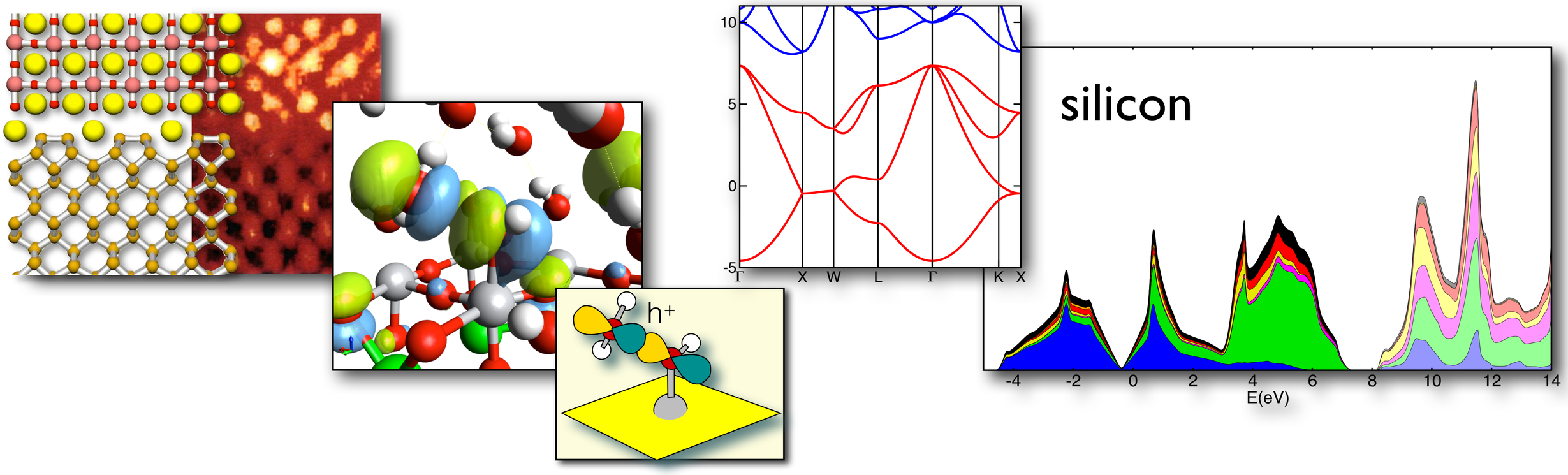
Hands-on course on first-principles calculations

Learn to perform ab-initio calculations of molecules and solids

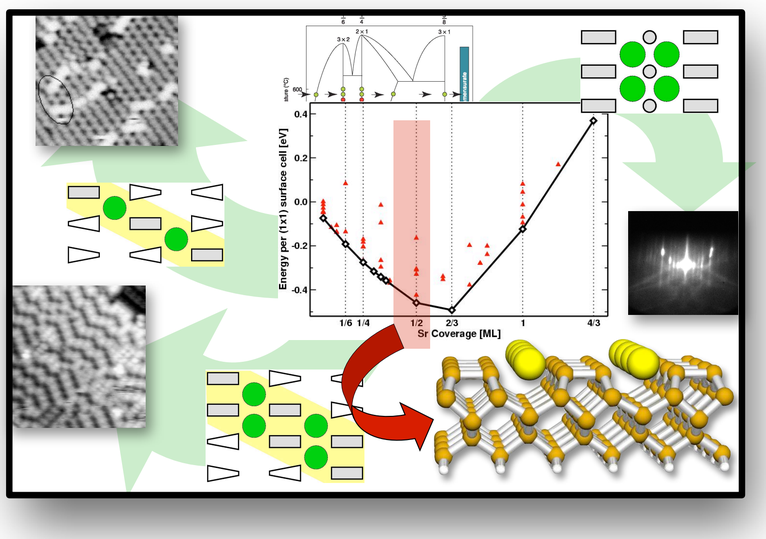


Time: 14-18 September 2015
Place: Göttingen University
Format: lectures and computer-hands-on
ECTS: 3 credits
Organizer: P.E. Blöchl
Contact: robert.schade@tu-clausthal.de
WWW: www2.pt.tu-clausthal.de/atp/handson.html
Apply: send email to robert.schade@tu-clausthal.de



Theoretical basis of first-principles calculations.
density-functional theory, ab-initio molecular dynamics, electronic structure methods

Understanding electronic structure and chemical bonds
patterns of bonding, from bonds to bandstructures, from atoms to solids, basics of magnetism.

Practice course using the CP-PAW code package
Step-by-step introduction under the guidance by experienced tutors.

Courses will be accompanied by detailed course materials.