TP 4

Chalkogenid-Schichtstrukturen: Wachstum und Grenzflächenphänomene

Theoretische Analyse der elektronischen und geometrischen Struktur von Festkörperoberflächen und die Bedeutung für Präparation und Wachstum von geschichteten Systemen

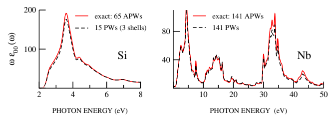
E.E. Krasovskii, C. Ramírez, O. Tiedje und W. Schattke

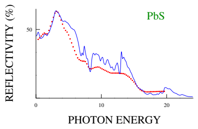
Ergebnisse / Fortsetzung

Theoretische Entwicklung

Methodologie: ELAPW-kp ISOLDA Code[1)]

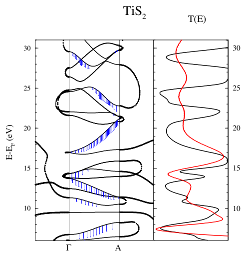
Ebene-Wellen-Darstellung der All-Elektronen-Wellenfunktionen





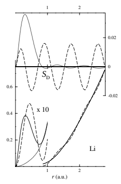
DK: erste Rechnung mit relativistischen Effekten und lokalen Feldeffekten[2)]

LEED/TCS



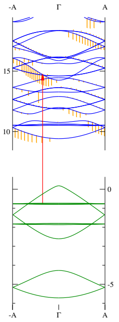
Halbraum-Variationsverfahren für Streuzustände

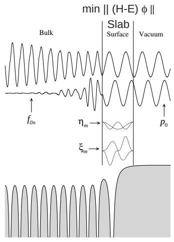
DFT: Gesamtenergie



AFC gouging

One-step Photoemission





- neuer Zugang zur Gesamtenergie durch AFC
- Orthogonalized ELAPW für große Einheitszellen

Entwicklung des slab-Codes und Vereinigung mit der Halbraummethode für Spektroskopie und Transportprobleme

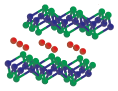
Selbstenergie

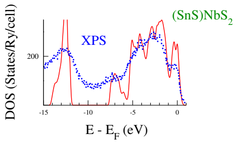
Zusammenarbeit: Blügel, Chulkov

- Superzelle: Gap ✓
- Halbraum Dispersion ✓
- Slab: dispersionslose Bänder ✓

Geordnete Schichtstrukturen

KCu_2Se_2



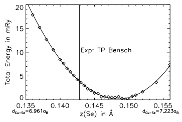


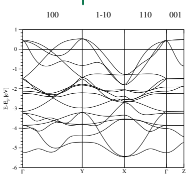
Fragestellungen:

- Schichtstruktur
- gemischte Valenzen
- Phasenübergang

X-ray und Synthese:

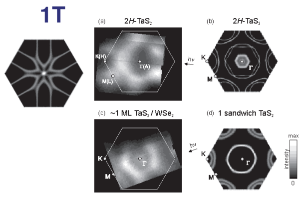
→ TP 1 Bensch





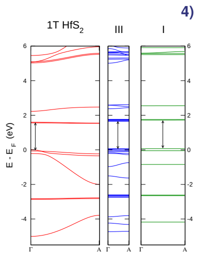
TaS_2 : Fermifläche[3)]

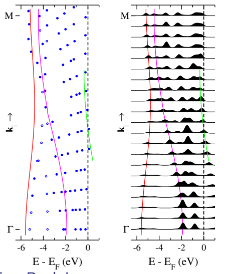
→TP 5 Kipp/Ski



$NbSe_2$

→ TP 5 Kipp/Ski [2,5)]
→ TP 12 Winkler





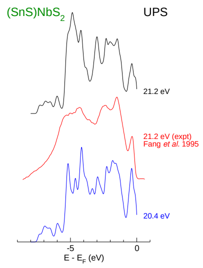
Exp. Peak-Lagen der Photoemission

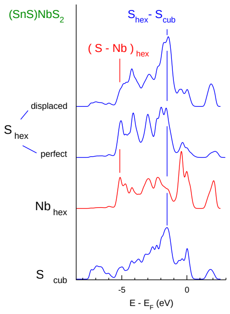
Theorie: Zustandsdichte

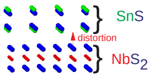
→ TP 3 Stettner
→ TP 7 Berndt
→ TP 5 Kipp/Ski
→ TP 10 Magnussen
→ TP 11 Tuczek

Misfitstrukturen[2)]

Defekte und Mittlung







elektronische Struktur (DOS etc.)

große Moleküle

(z.B. Aromat. KW, Alkylamine, Metallkomplexe)

Monolagen-Bedeckung, isolierte Adsorbate

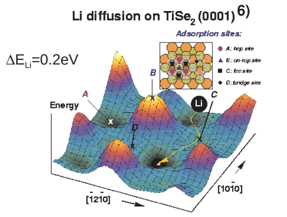
Geometrie

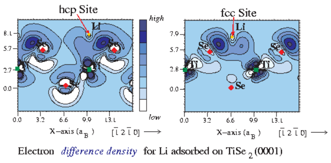
Vorarbeiten / Neuantrag

Oberflächen - DFT - Energieminimierung

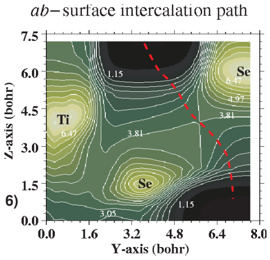
fhi98md

Li diffusion on $TiSe_2$ (0001) [6)]

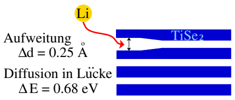




Electron *difference density* for Li adsorbed on $TiSe_2$ (0001)

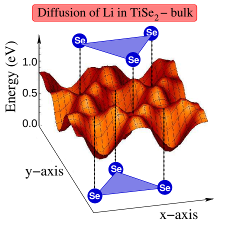


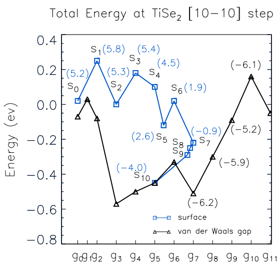
→ TP 5 Kipp/Ski[7)]



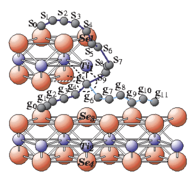
→ TP 1 Bensch

Diffusion of Li in $TiSe_2$ – bulk

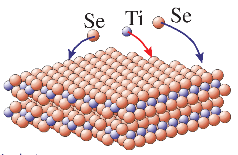




Li-Interkalation durch eine Stufe: negative Schwoebel-Barriere

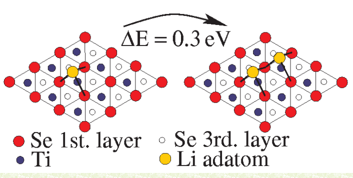


Elementares Wachstum



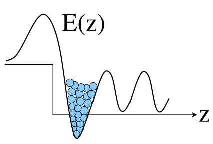
MBE-Wachstum
Diffusionsenergien
LDOS

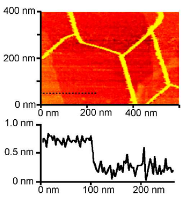
Adsorption und Interkalation mehrerer Atome



Drahtwachstum

Metall-Drähte, Inseln (Cu, Au, Alkali)
Schwoebel-Barriere
Bindung und Diffusion an Stufen





→ TP 5 Kipp
→ TP 7 Berndt
→ TP 6 Adelung
→ TP 8 Jäger

Rb/$TiTe_2$
Cu/VSe_2

fhi98md, SIESTA

1) E.E. Krasovskii and W. Schattke, Phys. Rev. B **63**, 235112 (2001)
2) E.E. Krasovskii et al., J. Electron Spec. Rel. Phen. **114-116**, 1133 (2001)
3) K. Rossnagel et al., Phys. Rev. B **63**, 125104 (2001)
4) M. Traving et al., Phys. Rev. B **63**, 035107 (2001)
5) J. Brandt et al., J. Electron Spec. Rel. Phen. **114-116**, 555-561 (2001)
6) C. Ramírez and W. Schattke, Surface Science **482-485**, 424-429 (2001)
7) R. Adelung et al., Phys. Rev. Lett. **86**, 1303-1306 (2001)

Veröffentlichungen (TP 4)