Metal adatom structures on semiconductor surfaces: Model systems for low-dimensional quantum matter

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• Tomonaga-Luttinger physics in 1D
• (non)Rashba physics in 2D
• Mott-Hubbard physics in a 2D triangular lattice
• Elemental topological insulator
Surfaces as "Quantum Simulators"

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The Würzburg "nanoteam" and friends

SR experiments
L. Patthey (SLS/PSI)
X.Y. Cui
J.H. Dil (U Zürich/EPFL/PSI)
B. Slomski
F. Meier
Eli Rotenberg (ALS)
A. Bostwick
J.L. McChesney

LT-STM
R. Matzdorf (U Kassel)
S. Mietke

Theory
W. Hanke (U Würzburg)
A. Fleszar
Gang Li
S.C. Erwin (Naval Research Lab)

work supported by DFG
Transition metal oxides
- Mott-Hubbard physics

Bechgaard salts:
- CDW/SDW instabilities
- Tomonaga-Luttinger liquid

ET-salts:
- magnetic frustration
- spin liquid behavior
ARPES

angle-resolved photoelectron spectroscopy

→ density of states
→ band structure
→ single-particle spectral function

\[ I_{PE} \propto A(\vec{r}, E) \]

STM/STS

scanning tunneling microscopy/spectroscopy

→ topographic/electronic imaging
→ local density of states
→ local single-particle spectral function

\[ dI_T/dU \propto A(\vec{r}, E) \]

BUT:
highly surface sensitive, probing depth: a few Å only!
Transition metal oxides
- Mott-Hubbard physics

Bechgaard salts:
- CDW/SDW instabilities
- Tomonaga-Luttinger liquid

ET-salts:
- magnetic frustration
- spin liquid behavior
Alternative approach: surfaces as model systems

Example: metal adatom (sub)monolayers on semiconductor surfaces

- epitaxial and self-assembled growth of 2D and 1D structures
- control and tunability: - substrate orientation
  - adatom/substrate combination
  - doping by coadsorption
  - ...

→ model systems with "tunable" electronic and magnetic properties
Atomic nanowires:
Au/Ge(100)
Interacting electrons in 1D
→ breakdown of the Fermi liquid concept
→ spin-charge separation
→ Tomonaga-Luttinger liquid as new paradigm
→ suitable materials for TLL behavior?

classical interaction in 1D: fatal
Interacting electrons in 1D

→ breakdown of the Fermi liquid concept
→ spin-charge separation
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Realization: anisotropic crystals

e.g., organic CT salts: TTF-TCNQ

PRL 88, 096402 (2002)
Interacting electrons in 1D
→ breakdown of the Fermi liquid concept
→ spin-charge separation
→ Tomonaga-Luttinger liquid as new paradigm
→ suitable materials for TLL behavior?

Realization: Au atom chains on Ge(100)
Interacting electrons in 1D

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Realization: Au atom chains on Ge(100)
Atomic nanowires: Au/Ge(100)

ARPES:
1D Fermi surface and "band" dispersion

PRB 83, 121411(R) (2011)
Atomic nanowires: Au/Ge(100)

STM: differential tunneling conductivity

→ gradual depression of spectral weight at zero bias

→ no structural or CDW phase transition below 585 K
Atomic nanowires: Au/Ge(100)

- absence of CDW down to 4 K
- power-laws and scaling: spectrum $\sim |E|^\alpha$, $\sim |T|^\alpha$
  \[ \rightarrow \text{Tomonaga-Luttinger liquid} \]
- exponent $\alpha$ of tunneling spectroscopy consistent with PES

Atomic nanowires: Au/Ge(100)

**differential tunneling conductivity**

![Differential tunneling conductivity graph]

**scaled conductivity**

![Scaled conductivity graph]

TLL scaling behavior:

\[
\frac{dI}{dV} \propto T^\alpha \cosh \left( \frac{eV}{kT} \right) \Gamma \left( 1 + \frac{\alpha}{2} + i \frac{eV}{2\pi kT} \right)^2 \otimes \frac{df}{dE}
\]

Atomic nanowires: Au/Ge(100)

Playing the surface playground:
- "bounded Luttinger liquid": chain end effects?
- effect of local impurities
- dimensional crossover: 1D $\rightarrow$ 2D
- carrier doping
- ...

Au epitaxy
Power law exponents in TLL theory (charge stiffness $K_\rho = 0.26$)

bulk: $\alpha_{bulk} = \frac{1}{4} (K_\rho + K_\rho^{-1} - 2) = 0.53$

chain end: $\alpha_{end} = \frac{1}{2} (K_\rho^{-1} - 1) = 1.42$

Other examples of atomic nanowires

Au/Si(hhk)

Au double chains

spin-polarized Rashba bands

Antibonding

Bonding

Au bands
Other examples of atomic nanowires

Au/Si(hhk)

"silicene nanoribbons" (cf. graphene)
Other examples of atomic nanowires

Au/Si(hhk)

silicene nanoribbons (cf. graphene)

DFT:
extra electron @ very 3rd Si edge atom
with local moment and AFM order

spin-integrated STM:
confirms theory
PRL 111, 137203 (2013)
Other examples of atomic nanowires

Au/Si(hhk)

In/Si(111) prototypical CDW system

H.W. Yeom et al. (1999)

→ following talk
Revolving spins: 
Au/Ge(111)
Revolving spins: Au/Ge(111)

Molecular Beam Epitaxy

Sub Monolayer Growth

Hot Deposition Technique

Ge/Si/InSb

Substrate Material and Orientation

(111)

(100)

Fe, Sn, Au, Pt
Spintronics without magnetism?

→ spin-orbit coupling at surface: Rashba effect

→ search for Rashba-split metallic surface states on insulating substrate

Realization: $\sqrt{3} \times \sqrt{3}$ Au/Ge(111)
Revolving spins: Au/Ge(111)

ARPES: mapping of bands and Fermi surface

→ metallic surface state on a semiconducting substrate
Revolving spins: Au/Ge(111)

ARPES
SIS beamline, SLS

band dispersions

Fermi surface

PRB 83, 235435 (2011)
Revolving spins: Au/Ge(111)

ARPES
SIS beamline, SLS
band dispersions

band theory
LDA+SIC

spin-orbit splitting

PRB 83, 235435 (2011)
Revolving spins: Au/Ge(111)

ARPES
SIS beamline, SLS

band dispersions

Fermi surface

PRB 83, 235435 (2011)
Revolving spins: Au/Ge(111)

Fermi surface
spin-resolved LDA

spin-integrated ARPES
Revolving spins: Au/Ge(111)

Fermi surface
spin-resolved LDA

3D spin-resolved ARPES
COPHEE @ SIS beamline, SLS

PRL 108, 186801 (2012)
Revolving spins: Au/Ge(111)

→ non-Rashba behavior: in- and out-of plane spin rotations
→ similar to topological insulators

3D spin-resolved ARPES
COPHEE @ SIS beamline, SLS

experimental SARPES spin vector results
non-Rashba behavior: in- and out-of plane spin rotations

similar to topological insulators
Spin texture of Au surface bands: striking similarity to the Dirac state of the topological insulator $\text{Bi}_2\text{Te}_3$

$$H(\vec{k}) = \left(\frac{\hbar^2 k^2}{2m^*} - C + c_h(k^6_+ + k^6_-)\right)\sigma_0 + v(k_x\sigma_y - k_y\sigma_x) + \lambda(k^3_+ + k^3_-)\sigma_z + i\zeta(k^5_+\sigma_- - k^5_-\sigma_+)$$

Fu, PRL 2009: DFT: Hexagonal Warping in $\text{Bi}_2\text{Te}_3$

Basak, PRB 2011: DFT: Radial Rotation in $\text{Bi}_2\text{Te}_3$

Isotropic Rashba term

Hexagonal warping and spin-z component

Radial rotation of planar spin

Revolving spins: Au/Ge(111)
Physics of frustration: Sn/Si(111)
Problem:

magnetic frustrations of local spin-1/2 moments on a triangular lattice

→ spin liquid?
→ 120° AFM Néel order?
→ other ordered states?

Realization: $\sqrt{3} \times \sqrt{3}$ Sn/Si(111)
Physics of frustration: Sn/Si(111)

**band theory**
w/o correlations ($U=0$)

![Band structure](image)

Sn 5p_z

metal
(1/2 filled)

**ab-initio many-body theory**
(LDA + DCA with $U=0.66$ eV)

![ARCES](image)

G. Li et al., PRB 83, 041104 (2011)

scanning tunneling spectroscopy (STS)

J. Settelein et al.

Mott insulator

LHB

UHB
local moments $\rightarrow$ magnetic ordering?
e.g., 120° Néel order

$\rightarrow$ band backfolding for 3x3 SDW
Physics of frustration: Sn/Si(111)

**band theory**

w/o correlations ($U=0$)

G. Li et al., PRB 83, 041104 (2011)

**ab-initio many-body theory**

(LDA + DCA with $U=0.66$ eV)

G. Li et al., Nat. Comm. 4, 1620 (2013)

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- Sn 5p₂
- metal (1/2 filled)

ARPE$^+$ "shadow bands"
Physics of frustration: Sn/Si(111)

Magnetic susceptibility $\chi(\vec{q})$ for triangular Hubbard model

$\rightarrow$ row-wise antiferromagnetic order

stabilized by long-range single particle hopping $t_{nnn}$

+ 3fold domain structure
Physics of frustration: Sn/Si(111)

Direct comparison of ARPES with DCA spectral function

→ confirms (short-range) collinear AF row-wise order

Nat. Comm. 4, 1620 (2013)
Direct comparison of ARPES with DCA spectral function

→ confirms (short-range) collinear AF row-wise order

next step:

– search for local moments by spin-resolved STM

– problem: moment predicted to be small ($\mu_{Sn} \approx 0.06 \mu_B$)
Physics of frustration

Isotropic triangular Hubbard model

example: superconductivity in Pb/Si(111)

Playing the surface playground:

- group IV atoms on (111) surfaces: Sn, Pb on Si(111), Ge(111)
- tuning of correlation, bandfilling, spin-orbit coupling
- topological superconductivity?
- ...

Uchihashi et al., PRL (2011)
Topological insulators go elemental: \( \alpha \)-Sn/InSb(001)
Topological insulators (TIs)

- Spin-orbit coupling + band-inverted insulator
- Conducting and spin-polarized surface/edge states in the gap

3D TIs with 2D surface states

2D TIs with 1D edge states

known 3D topological insulators:

- $\text{Bi}_2\text{X}_3$ (X=Se, Te)
- strained HgTe /CdTe(001)
- ...
known 3D topological insulators:

- $\text{Bi}_2\text{X}_3$ (X=Se, Te)
- strained HgTe /CdTe(001)
- ...
known 3D topological insulators:
• Bi$_2$X$_3$ (X=Se, Te)
• strained HgTe /CdTe(001)
• ...

predicted:
• strained α-Sn /InSb(001)
ARPES: topological surface states and Dirac cone
Identification of the topological character: spin-polarized ARPES
TIs go elemental: $\alpha$-Sn/InSb(001)

**Doping effects:**
- intrinsic p-doping by In diffusion
- counter-doping with Te, acts also as surfactant
Sn as 2D topological insulator: stanene

Stanene = Sn bilayer (cf. graphene)

Control parameters:
- strain
- dangling bond saturation (sp² vs. sp³)
Metal adatoms on semiconductor surfaces as Quantum Simulators

- experimentally well-controlled
- "tunable" properties
- ideally suited for ARPES and STM/STS

- examples:
  - Fermi liquid breakdown in 1D
  - (non-)Rashba physics in 2D
  - Mott-Hubbard physics in frustrated geometries
  - elemental topological insulator

- perspectives:
  - doping/bandfilling effects
  - 1D-2D crossover
  - spin-orbit coupling
  - topological physics
  - ...

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