High Energy and Momentum Resolved Photoemission Studies of Quasi-One-Dimensional Blue Bronze K$_{0.3}$MoO$_3$

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Outline

Introduction:
✓ Crystal structure
✓ Electronic structure
✓ Structural studies of Charge Density Waves

Experimental details:
✓ Photoelectron spectrometer

Experimental data:
✓ Band structure of \( \text{K}_{0.3}\text{MoO}_3 \)
✓ Fermi wave vectors versus temperature
✓ Commensurate to incommensurate CDW transition
Low dimensionality $\Rightarrow$ (i) Charge Density Waves (CDW), Peierls transitions
(ii) Electron correlation effects
/Non-Fermi liquid behavior, spin-charge separation, HTC/

J.-P. Pouget et al., J. Physique Lett. 44, L113 (1973)
Electronic structure of $K_{0.3}MoO_3$

/tight-binding calculations/


Two chains per unit cell $\Rightarrow$ two bands crossing the Fermi level

How many Charge Density Waves?
Structural studies of CDW in K$_{0.3}$MoO$_3$

/Single Charge Density Wave/

(i) Diffuse X-ray scattering

\[ q_{CDW} = 2k_F b^x / \]

J.-P. Pouget et al.

(ii) Temperature dependent neutron scattering

/commensurate to incommensurate transition/

M. Sato, H. Fujishita and S. Hoshito,

Nesting:
Fermi surface of the first band is nested to the Fermi surface of the second band

CDW wave vector

\[ q_{CDW} : k_{F1} + k_{F2} \]
Temperature dependence of CDW wave vector:

◊ Thermally activated charge transfer between bands crossing the Fermi level and third band above it
   /Pouget et al./

◊ Shift of the chemical potential
   /Pouget & Nougera, Artemenko et al./

◊ Hidden temperature dependence of the nesting vector
   /Intention of the present study/

Goals of photoemission experiment:

◊ Direct monitoring $k_{F_1}$ and $k_{F_2}$
◊ Temperature dependence of $(k_{F_1}+k_{F_2})$
Photoelectron Spectrometer
/Gammadata, SES-200/

✓ Multichannel detection in emission angle and kinetic energy

✓ Energy resolution ~ 10 meV

✓ Angle resolution ~ 0.2°

✓ Base pressure ~ 2 × 10^{-11} Torr

Presently located at the U13UB beamline at the National Synchrotron Light Source, BNL
Example of photoemission data

$3$-D maps of photocurrent/

Experimental details:

Samples cleaved \textit{in situ}

Liquid He cryostat provides temperatures from 
$\sim$20 K to $\sim$450 K

Temperature monitored with a help of OMEGA CY7 sensor
Momentum Distribution Curves at $E_F$

Intensity at the Fermi level

Electron Momentum along $\Gamma X$ (Å$^{-1}$)

$T=300$ K

$T=200$ K

$T=180$ K

$T=150$ K

$T=120$ K

$T=100$ K

$T=80$ K

$T=62$ K

$T=40$ K
Commensurate to incommensurate CDW transition in $K_{0.3}MoO_3$
/comparing neutron scattering data with nesting vector measured in photoemission experiment/

$1-|k_{F1} + k_{F2}|$ and $1-q_{CDW}$ (b$^\times$ units)

Temperature (K)

Present work

Neutron scattering,
Fermi surface of an array of coupled chains
/tight binding calculation/

Fermi surface is given by:

\[ \mu = -2\cos(k_{//}) \pm (t_{//} + 2t_{//} t \cos(k_{//})+t)^{\sigma} \]