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Electron Transport in Se-Doped LT-TaS2

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unambiguous symmetry assignment for the two-photon transition (\(\lambda_{-}\lambda_{+}\)), and absolute oscillator strengths for both the one-photon and two-photon transitions (0.8 and 1.5 respectively). Cross sections for two-photon absorption in polyacetylene are by far the largest ever reported for an organic molecule (\(10^{-46} \text{ cm}^2\text{-sec-photon-repeat unit}\)). These remarkably large values are quantitatively explained theoretically.  


SESSION JP: LAYERED COMPOUNDS I, TRANSPORT AND MAGNETIC PROPERTIES
Thursday morning, 22 March 1979
Great America Room II at 9:00 A.M.
S.A. Jackson, presiding

JP 1 "Direct" Observation of Charge Density Waves by Molecular Beam Diffraction
G. BIANCO, P. CAMERON, and L. COLILLI, University of Genoa, Italy
-- A diffraction pattern of neutral helium atoms (\(\lambda = 0.57 \text{ Å}\)) has been obtained from the surface of a \(\text{TaSe}_2\) single crystal at 80K. Cleavage of the surface was accomplished by heating up to 350-400K, and by cryopumping with liquid helium in proximity of the crystal. Satellite peaks are also observed in addition to the ordinary Bragg reflections, consistent with the \(3\text{a}/\lambda\) superstructure of the \(\text{TaSe}_2\) phase, expected at 80K. What is surprising is that, while in electron, neutron and x-ray diffraction the intensities of the satellite peaks are 20-50 times weaker than ordinary Bragg reflections, in this experiment they have about the same intensity. Since a molecular beam has no penetration whatsoever in the crystal our results are interpretable in terms of diffusion effects from the corrugated surface. What is observed, then, is most likely the direct effect of charge modulation in the electron sea, rather than the reaction of the positive ion lattice to the charge modulation.

On sabaitical leave from Purdue University, Physics Department, West Lafayette, IN 47907, U.S.A.

JP 2 Does \(\lambda\)-MoTe\(_2\) Have a CDW Instability? ROY CLARKE\*, P. WONG\*, and P.M. HORN, University of Chicago,** and E. MARSEGLIA, Cavendish Laboratory, Cambridge.-- The recently reported monoclinic-orthorhombic structural transition in \(\lambda\)-MoTe\(_2\) (quenched from the metallic, paramagnetic \(\text{MoTe}_2\) phase) is unusual in that the lower temperature phase has the higher symmetry. We present magnetic susceptibility measurements which show that \(\lambda\)-MoTe\(_2\) is diamagnetic at 300K and that \(\lambda\) exhibits a gradual downward step going into the orthorhombic phase with thermal hysteresis over a wide temperature range. Although there is as yet no direct evidence of charge density wave (CDW) formation in \(\lambda\)-MoTe\(_2\) the results suggest a possible explanation for the transformation in which a competition between Coulomb and elastic interactions drives a first-order lock-in transition to the orthorhombic phase below 250 K.

**Supported by NSF, Materials Research Laboratory, University of Chicago.

1) R. Clarke, E. Marsegilia, and H.P. Hughes, Phil. Mag. 38, 121 (1978)

JP 3 Angle-Resolved Photoemission Studies of the Band Structure of \(\text{TaS}_2\) and \(\text{TaSe}_2\).
C. J. ADKINS, P. M. HOWELL, R. H. WALLIS, and M. KAPOK, University of Wisconsin-Madison, F. LEVY, Institut de Physique Appliquee, INP, Lausanne, Switzerland, and J. BARRUTI, Istituto di Fisica del Politecnico, Milano, Italy.-- We have carried out a systematic study of \(\text{GaS}_2\)-\(\text{Se}_x\) compounds in the range \(x = 0.1-1\) employing photoemission spectroscopy with synchrotron radiation. The atomic orbital character of each valence band peak is reflected in the dependence on \(x\) of its binding energy (measured with respect to the top of the valence band). For example the \(p_z\)-like states near the top of the valence band are shifted downwards by \(0.25 \text{ eV}\) when \(x\) is changed from 1 to 0. On the contrary the \(p_x\) states are shifted upwards by \(0.25 \text{ eV}\). For large values of \(x\) the photon polarization dependence of these peaks reveals a hybridization of the \(p_z\) and \(p_x\) states. The Ga \(3d\) binding energy also decreases linearly with \(x\), an effect clearly revealed by previous measurements on GaS and GaSe. The above composition effects and the dependence on \(x\) of other valence band peaks will be discussed in terms of the chemical bonding properties of these materials.

JP 4 Composition-Dependent Binding Energies in \(\text{GaS}_2\)-\(\text{Se}_x\) Compounds
G. MARGARITONDO, A.D. KURNIT and T.E. MILLIGAN, Dept. of Physics, University of Wisconsin-Madison, F. LEVY, Institut de Physique Appliquee, INP, Lausanne, Switzerland, and I. BARRUTI, Istituto di Fisica del Politecnico, Milano, Italy.-- We have carried out a systematic study of \(\text{GaS}_2\)-\(\text{Se}_x\) compounds in the range \(x = 0.1-1\) employing photoemission spectroscopy with synchrotron radiation. The atomic orbital character of each valence band peak is reflected in the dependence on \(x\) of its binding energy (measured with respect to the top of the valence band). For example the \(p_z\)-like states near the top of the valence band are shifted downwards by \(0.25 \text{ eV}\) when \(x\) is changed from 1 to 0. On the contrary the \(p_x\) states are shifted upwards by \(0.25 \text{ eV}\). For large values of \(x\) the photon polarization dependence of these peaks reveals a hybridization of the \(p_z\) and \(p_x\) states. The Ga \(3d\) binding energy also decreases linearly with \(x\), an effect clearly revealed by previous measurements on GaS and GaSe. The above composition effects and the dependence on \(x\) of other valence band peaks will be discussed in terms of the chemical bonding properties of these materials.

JP 5 Resistivity of \(\text{Zr}_{1-x}\text{Ti}_x\text{Se}_2\) and \(\text{Zr}_{1-x}\text{Ti}_x\text{S}_2\)
W.R. NIEVEEN and R.D. KIRBY, U. of Nebraska.--Pure \(\text{TiSe}_2\) shows a large resistivity peak near 200 K arising from a second-order transition to a charge-density-wave (CDW) state. Our resistivity measurements on \(\text{Zr}_{1-x}\text{Ti}_x\text{Se}_2\) show that the CDW transition temperature shifts downward with increasing \(x\). By \(x = 0.3\), the CDW transition is suppressed, and the resistivity can be characterized by a simple power law dependence: \(\rho = (\rho_0 x)^{-1/3}\). This expression holds for temperatures between 20 K and 300 K. Wilson has suggested that the unusual temperature-dependent resistivity of \(\text{ZrSe}_2\) (where an \(\alpha T^3\) dependence was found) is due to scattering of carriers by homopolar optic phonons. Our results on \(\text{Zr}_{1-x}\text{Ti}_x\text{Se}_2\) are consistent with this picture.

*Work supported by the NSF under grant DMR 77-10217.

Present Address: Materials Science Center, Northwestern University.


5) P. Fazzekas and E. Rosatti (private communication).