KOND

Tuesday, 10.09.2024, Room ETZ E 7

Time	ID	**KOND I: Coupled degrees of freedom** *Chair: Thomas Greber, Universität Zürich*
14:00	**101**	**Coupled magnetism and ferroelectricity in magnetic high entropy oxide** *Roxana Capu [1], Subhrangsu Sarkar [2], Ryan Thompson [2], C. Willem Rischau [3], Marli R. Cantarino [4], Stefan Schuppler [5], Sergey Budko [6], Stefano Gariglio [3], Zaher Salman [7], Yurii Pashkevich [2,8,9], Christian Bernhard [2]* *[1] West University of Timisoara, Romania,* *[2] Department of Physics, University of Fribourg, CH-1700 Fribourg, [3] Université de Genève,* *[4] ESRF, Grenoble, France,* *[5] Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology (KIT), Germany* *[6] Ames Laboratory, U.S.A, [7] Paul Scherrer Institut* *[8] Fribourg Center for Nanomaterials, University of Fribourg, CH-1700 Fribourg* *[9] O. Galkin Donetsk Institute for Physics and Engineering, NAS of Ukraine* Using low energy Muons spin rotation spectroscopy, measurement of dc/ac magnetic susceptibility and measurement of capacitance, we show that epitaxially grown Nd-based perovskite high entropy oxides exhibit significant ferromagnetism, spin-glass behaviour, high dielectric constant at RT and a temperature-dependent ferroelectric hysteresis that are intricately coupled to each other. X-ray absorption spectroscopy at 3d transition metal edges indicates a mixed valence state – possibly originating from the off-centring of the B-sites – that helps to explain these properties. These materials could be useful for exploiting magnetostriction and other related properties leading to next-generation sensors.
14:15	**102**	**Terahertz electric-field-driven dynamical multiferroicity in $SrTiO_3$** *Martina Basini [1], Matteo Pancaldi [2], Björn B. Wehinger [3], Alexander V. Balatzky [4,5], Stefano Bonetti [6], Matthias C. Hoffmann [7], Terumasa Tadano [8], Mattia Udina [9], Vivek Unikandanunni [10]* *[1] ETH Zürich, Physics Department, [2] Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Italy* *[3] European Synchrotron Radiation Facility, Grenoble, France, [4] NORDITA, Stockholm, Sweden* *[5] Department of Physics, University of Connecticut, Storrs, CT, USA* *[6] Department of Molecular Sciences and Nanosystems, Ca'Foscari University of Venice, Italy* *[7] Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, CA, USA* *[8] Research Center for Magnetic and Spintronic Materials, National Institute for Materials Science, Tsukuba, Japan* *[9] Department of Physics and ISC-CNR, 'Sapienza'University of Rome, Italy* *[10] Bern University* The emergence of collective order in matter is among the most fundamental and intriguing phenomena in physics. Recently, the theoretical concept of dynamical multiferroicity has been introduced to describe the emergence of magnetization due to time-dependent electric polarization in non-ferromagnetic materials. Here we provide experimental evidence of room-temperature magnetization in the archetypal paraelectric perovskite $SrTiO_3$ due to this mechanism. We resonantly drive the infrared-active soft phonon mode with an intense circularly polarized terahertz electric field and detect the time-resolved magneto-optical Kerr effect. Our findings show a new path for the control of magnetism, for example, for ultrafast magnetic switches, by coherently controlling the lattice vibrations with light.

14:30	103	**Phonon-Polariton Nonlinearities in Ferroelectric $LiNbO_3$** *Rossella Acampora [1], Megan Biggs [2], Elsa Abreu [1], Jeremy Johnson [2], Steven Johnson [1]* *[1] ETH Zürich, [2] BYU* In ferroelectric $LiNbO_3$, THz light couples with low-frequency optical phonons and form phonon polaritons. Recent studies have shown that is possible to probe nonlinearities at specific points along the phonon-polariton dispersion curve with different probe wavelengths after broadband excitation with strong THz transients. However, extensive measurements of lattice anharmonicities in $LiNbO_3$ are still lacking. To bridge this gap, we characterised the nonlinear behaviour of phonon-polaritons in $LiNbO_3$ using nonlinear THz spectroscopy. We mapped the $LiNbO_3$ phonon polariton E branch by varying the probe wavelength and observed a strong dependence of the nonlinear response on the wavelength of the near-optical pulse, which arises from the momentum selection of the detection process.
14:45	104	**Strong enhancement of superconductivity in fractal lattices** *Askar Iliasov [1], Andrey Bagrov [2], Mikhail Katsnelson [2]* *[1] University of Zurich, [2] Radboud University* Using the Sierpinski gasket as an example, we theoretically study the properties of fractal superconductors. We focus on the phenomenon of s-wave superconductivity in the Hubbard model with attractive on-site potential and employ the Bogoliubov-de Gennes approach. For the case of the Sierpinski gasket, we demonstrate that fractal geometry of the underlying crystalline lattice can be strongly beneficial for superconductivity, not only leading to a considerable increase of the critical temperature as compared to the regular triangular lattice but also supporting macroscopic phase coherence of the Cooper pairs.
15:00	105	**Decoupled static and dynamical charge correlations in $La_{2-x}Sr_xCuO_4$** *Leonardo Martinelli [1], Izabela Biało [1], Johan Chang [1], Jaewon Choi [2], Mark Fischer [1], Mirian Garcia-Fernandez [2], Xunyang Hong, Tohru Kurosawa [3], Chun Lin [1], Migaku Oda [4], Jens Oppliger [1], Qisi Wang [5], Ke-Jin Zhou [2]* *[1] University of Zurich, [2] Diamond Light Source, [3] Muroran Institute of Technology* *[4] Hokkaido University, [5] The Chinese University of Hong Kong* The physics of charge order in high-temperature superconducting cuprates is still largely unexplained. Recent experiments revealed the presence of strong quantum fluctuations, whose doping and temperature dependence suggest the closeness to a quantum critical point and a relation to the strange-metal phase. We used ultra-high-resolution Resonant Inelastic X-ray Scattering in combination with uniaxial strain to investigate the stripe-ordered cuprate $La_{2-x}Sr_xCuO_4$. This allowed us to investigate the properties of the associated quantum fluctuations and phonon softening in an artificially detwinned striped state. We discover a clear connection between quantum charge fluctuations and bond-stretching phonons, and an apparent de-coupling between the static charge order and its fluctuations, which display a different symmetry.
15:15	106	**Investigation of the phase transition driven by ultrashort laser pulses in the charge-density-wave material $K_{0.3}MoO_3$** *Rafael T. Winkler [1], Elsa Abreu [1], Christopher Arrell [2], Danylo Babich [2], Paul Beaud [2], Simone Biasco [1], Larissa Boie [1], Jure Demsar [3], Yunpei Deng [2], Edwin J. Divall [2], Sabina Gurung [1], Steven Johnson [1], Henrik Lemke [2], Roman Mankowsky [2], Abhishek Nag [2], Samuel Norton [1], Alexander R. Oggenfuss [2], Vladimir Ovuka [1], Mathias Sander [2], Matteo Savoini [1], Davide Soranzio [1], Urs Staub [2], Tim Suter [1], Janine Zemp (Dössegger) [1], Serhane Zerdane [2]* *[1] ETH Zürich, [2] SwissFEL, Paul Scherrer Institute, Villigen,* *[3] Faculty Institute of Physics, Johannes Gutenberg-University Mainz* Blue Bronze ($K_{0.3}MoO_3$) is a quasi 1D material exhibiting a charge-density-wave (CDW) with a periodic lattice distortion (PLD). In a time resolved x-ray experiment at SwissFEL, we study the dynamics of the PLD by pumping $K_{0.3}MoO_3$ with short laser pulses and probing it using x-ray diffraction. We construct reciprocal space maps (RSM) of superlattice reflections at different delays. The RSMs indicate a transient but not persistent flip of the phase of the CDW. We attribute the suppression of the diffracted x-ray intensity after this flip to a fast decoherence of the CDW driven by pinning of the phase of the CDW in the material indicating an order-disorder like phase transition.

15:30	**107**	**Resonant Ultrasound Spectroscopy Study of the Vortex Lattice Phase Diagram of Niobium** *Xuan Dang Dang, Jonas Philippe, Marek Bartkowiak, Marc Janoschek, Paul Scherrer Institut* Here, we will present the development of a novel resonant ultrasound spectroscopy (RUS) setup. Subsequently, we report our investigation of the superconducting vortex lattice of a commercially available single crystal of high purity (Nb - 99.999%). Based on our measurements, we determine the vortex lattice phase diagram, and compare it to results from electrical resistivity and neutron scattering studies.
15:45	**108**	**Tuning the Electronic Properties of Two-Dimensional Lepidocrocite Titanium Dioxide-Based Heterojunctions** *Kati Asikainen, Matti Alatalo, Marko Huttula, Assa Sasikala Devi, University of Oulu* This study investigates a 2D Janus heterostructure made by combining lepidocrocite TiO_2 and MoSSe, focusing on the energetic stability and change in electronic properties with respect to varied interface terminations. Using state-of-the-art density functional theory simulations, we show that TiO_2-MoSSe heterostructures are energetically feasible to form. The results indicate that by varying the atomic species at the interface, the electronic structure can be considerably altered due to the differences in charge transfer arising from the inherent electronegativity of the atoms. The work demonstrates that the Janus interface enables the tuning of electronic properties, providing an understanding of the possible applications of the TiO_2-MoSSe heterostructure.
16:00		***Coffee Break***
18:30		***CERN 70***
19:45		***Postersession with Apéro***

Thursday, 12.09.2024, Room ETZ E 7

Time	ID	**KOND II: Advances in Methodology** *Chair: Daniel Mazzone, PSI Villigen*
14:00	**111**	**Characterization of high-purity nickel single crystals by mechanical spectroscopy** *Anna Nastruzzi, Weibin Jiang [2], Daniele Mari [3], Manuel Pouchon [1,3]* *[1] PSI, [2] CAS, [3] EPFL* Mechanical spectroscopy tests of high-purity nickel single crystal, with different lattice orientations, were performed in a forced oscillation pendulum, under high vacuum, at different frequencies. The temperature was varied from room temperature up to 500 °C. A periodic strain of amplitude 5×10^{-5} was applied. Internal friction spectrum reveals 3 mechanical loss peaks: P0 (transient peak), P1 and P2. P1 and P2 might be related to a motion of dislocations controlled by the migration of 2 types of jogs. Activation energies in the range 1.5 - 2 eV were found for both P1 and P2 peaks. These are comparable to pipe diffusion. TEM analyses confirmed the presence of dislocation jogs.

14:15	**112**	**Imaging heat transport in suspended diamond nanostructures with integrated spin defects thermometers** *Valentin Goblot [1], Kexin Wu [1], Enrico Di Lucente [1], Elena Losero [1], Yuchun Zhu [1], Claudio Jaramillo [1], Nicola Marzari [1], Michele Simoncelli [2], Christophe Galland [1]* *[1] EPFL, [2] University of Cambridge* Diamond offers excellent prospects for the study of phonon transport phenomena beyond Fourier's law at room temperature. Here, we investigate heat transport properties of suspended diamond microstructures using NV centers in the diamond lattice as in-situ temperature sensors. We present diffraction-limited spatially resolved measurements of temperature across suspended cantilevers, with a temperature resolution below 100mK using frequency-modulated lock-in readout of the spin resonance. We extract the effective thermal conductivity of each cantilever and reveal a surprisingly steep dependence on the cantilever lateral dimension, highlighting the need for further experiments and theoretical refinement to fully understand boundary and confinement effects.
14:30	**113**	**Electronic Viscous Flow in Hexagonal Boron Nitride Encapsulated Graphene FETs** *Wenhao Huang, Michel Calame [1,2], Tathagata Paul, Mickaël Lucien Perrin [1]* *[1] Empa, [2] University of Basel* Conventional electron transport in conductors involves diffusive scattering and interactions with lattice vibrations, resulting in Ohmic behavior. However, a distinct regime arises when electron-electron interactions induce correlated, momentum-conserving flow akin to classical fluid dynamics. Our study delves into charge hydrodynamic transport, revealing width-dependent conductivity and reduced resistivity at higher electron temperatures. We observe charge vortices and validate viscous effects over a broad temperature range, including room temperature, particularly notable in graphene compared to other systems. Finite element calculations confirm our findings and suggest geometries to enhance viscous effects, promising applications like geometric rectifiers and charge amplifiers. This research advances our understanding and utilization of charge hydrodynamics in graphene-based systems.
14:45	**114**	**Laser induced structural dynamics in colloidal gold nanoparticles** *Changji Pan [1], Klaus Sokolowski-Tinten [2], Albert Thies [2], Laurenz Kremeyer, Anton Plech [3], Anna Ziefuss [2]* *[1] ETH Zürich, [2] University of Duisburg-Essen, [3] Karlsruher Institut für Technologie* Laser induced energy transfer and dissipation in nanoparticles within a liquid environment are of specific interest due to their relevance in photochemical and biomedical applications. In particular a quantitative understanding of electron-phonon coupling (EPC) is required for determining the life-time of hot electrons and heat generation. Currently, most related studies are based on optical pump-probe experiments, which only provide information related to electron dynamics. Here, we use time-resolved X-ray scattering at SwissFEL to characterize laser induced structural dynamics in colloidal gold nanoparticles. Our measurements provide direct and quantitative information on structural response, indicating a chemical environment-dependent EPC process.
15:00	**115**	**Ultrafast EBIC: A new technique for semiconductor device characterization with ps time resolution** *Joel Rehmann, Matthias Röllin, Nikolaus von Schickh, Francisco Carrion Ruiz, Andreas Vaterlaus, Yves Marc Acremann, ETH Zürich* For the first time we demonstrate an ultrafast scanning electron (USEM) microscope with electron-beam-induced current (EBIC) capability. This novel technique allows for in-situ observation of depletion layers in fast semiconductor devices. We demonstrate micrometer spatial and picosecond temporal resolution on an avalanche photodiode. EBIC is a well established method in semiconductor analysis. Paired with a pump probe approach in a USEM the method provides a new tool for developing milimeter-wave electronics.

15:15	**116**	**Growth by pulsed laser deposition of $SrVO_3$ thin films for optical applications** *Tancredi Thai Angeloni, Ian Aupiais, Andrea Caviglia, Stefano Gariglio, Alexey Kuzmenko, Clémentine Thibault, Javier Toboada-Gutierrez, University of Geneva* Light-matter interaction can be strongly enhanced by confining the electric field in optical cavities. These require a well-suited stacking of reflecting and transparent materials selected for the frequency range of interest. In our study, we target the Terahertz spectrum and have chosen the $SrVO_3$ compound for its high reflectivity in this frequency range. We report results on the growth of $SrVO_3$ thin films by pulsed laser deposition unraveling the complex dependence of resistivity and crystalline quality on the Ar/O_2 growth atmosphere as well as laser fluence and target-substrate distance. Optical measurements performed by Fourier Time-domain InfraRed spectroscopy show that the reflectivity window is within the scope of our applications.
15:30	**117**	**Increasing the dynamical range of a scanning tunneling microscope** *Ajla Karic, Carolina Marques, Fabian Natterer, University of Zurich* A method for increasing the dynamical range of scanning tunneling microscopes (STM) is introduced. We first transform the nonlinear current-voltage characteristic into a time-dependent current via AC excitation and then actively cancel dominant current harmonics using a driven compensating capacitor. The placement of the compensating capacitor allows us to create removal currents precisely opposing the currents that would otherwise saturate the preamplifier. Eliminating DC currents has no effect on the local density of states measurements, and removing the first harmonic only rigidly shifts the conductivity by a known amount.
15:45	**118**	**Analytical redefinition of the adsorbate-induced surface response of a metal** *Aleksandra Siklitskaya, Tomasz Bednarek, Adam Kubas, Institute of Physical Chemistry PAS* We introduce an innovative analytical framework for analyzing the interaction of charged perturbations with a three-dimensional (3D) half-infinite conductive space. Our method merges the quasi-3D expansion of the one-dimensional (1D) Kronig-Penney metal with Tamm's surface states, offering a comprehensive analysis tool for multipole molecule-conductive surface interactions. Validated against density functional theory (DFT) results on CO adsorption on Pt(111) slabs, our model accurately predicts changes in adsorption site preference with increasing coverage, aligning with experimental findings. Notably, our model maintains scalability with reported CO-CO interaction potentials on Pt(111) surfaces, reducing computational costs by a factor of 1000 compared to quantum chemical calculations, while delivering precise surface response solutions.
16:00		
16:30		***Coffee Break***
19:00		***Transfer to Dinner***
19:30		***Conference Dinner***

Friday, 13.09.2024, Room ETZ E 7

Time	ID	**KOND III: Many-body systems** *Chair: Aline Ramires, PSI Villigen*
	~~121~~	⇒ *moved to talk 13*
13:30	122	**Magnetostriction measurements of quantum spin ice candidates at ultra-low temperatures** *Ilaria Villa, Marek Bartkowiak, Michel Kenzelmann, Romain Franck Sibille, Paul Scherrer Institut* Rare-earth pyrochlores frequently exhibit spin ice correlations and, therefore, can potentially host quantum spin ice (QSI) phases. In these systems, the spin-orbital ground state doublet can be represented as an effective pseudo-spin 1/2. In addition to dipolar moments, multipoles are allowed, which can stabilise ice or ordered phases, or introduce quantum fluctuations on a dipolar spin ice manifold. Magnetostriction can reveal hidden multipolar orders and is proposed for distinguishing dipolar and octupolar QSI. This study presents magnetostriction measurements at ultra-low temperatures on QSI candidates based on cerium and praseodymium.
13:45	123	**Quantum Phase Transitions with a Lee-Yang Method and Many-Body Algorithms** *Pascal Vecsei, Christian Flindt, Jose L. Lado, Department of Applied Physics, Aalto University* Predicting the phase diagram of interacting quantum many-body systems is a central problem in quantum matter. Here, we show that a Lee-Yang method, combined with numerical quantum many-body methods such as matrix product states and neural network quantum states, can be used to investigate quantum phase transitions and predict the critical points of correlated spin and fermion models. Specifically, we implement our approach for quantum phase transitions in the transverse-field Ising model on different lattice geometries, as well as an interacting fermionic chain. As such, our results provide a starting point for determining the phase diagram of more complex quantum many-body systems.
14:00	124	**Hybrid Tree Tensor Networks for quantum simulation** *Julian Schuhmacher [1,2], Alberto Baiardi [2], Marco Ballarin [3], Giuseppe Magnifico [4], Simone Montangero [3], Francesco Tacchino [2], Ivano Tavernelli [2]* *[1] EPFL, [2] IBM Research Zurich, [3] University of Padova, [4] University of Bari* Hybrid Tensor Networks (hTNs) offer a promising solution for encoding variational quantum states beyond the capabilities of efficient classical methods or noisy quantum computers alone. However, their practical usefulness and many operational aspects of hTN-based algorithms have not been thoroughly investigated yet. In this contribution, we introduce a novel algorithm to perform ground state optimizations of hybrid Tree Tensor Networks (hTTNs), discussing its advantages and roadblocks. We benchmark our approach on two paradigmatic models, namely the Ising model at the critical point and the Toric code Hamiltonian. In both cases, we successfully demonstrate that hTTNs can improve upon classical equivalents with equal bond dimension in the classical part.
14:15	125	**Benchmarking digital quantum simulations and optimization above hundreds of qubits using quantum critical dynamics** *Alexander Miessen [1,2], Daniel Egger [1], Ivano Tavernelli [1], Guglielmo Mazzola [2]* *[1] IBM Quantum, IBM Research –Zurich, [2] Institute for Computational Science, University of Zurich* We utilize known theoretical results about many-body quantum critical dynamics to benchmark quantum hardware and various error mitigation techniques on up to 133 qubits. In particular, we benchmark against known universal scaling laws in the Hamiltonian simulation of a time-dependent transverse-field Ising Hamiltonian. Incorporating basic error mitigation and suppression, our study shows coherent control up to a two-qubit gate depth of 28, featuring a maximum of 1396 two-qubit gates, before noise becomes prevalent. These results are transferable to applications such as digitized quantum annealing and match the results of a 133-site optimization, where we identify an optimal working point in terms of both circuit depth and time step.

14:30 | **126**

Fractional Topological Insulators in Twisted Transition Metal Dichalcogenides

Glenn Wagner [1], Andrei Bernevig, Kouta Dagnino, Yves Kwan, Titus Neupert [2], Jiabin Yu
[1] ETH Zürich, [2] Universität Zürich

The recent experimental observations of fractional Chern insulators in moiré systems without an applied magnetic field prompt the question of whether their time-reversal invariant generalization, fractional topological insulators (FTIs), can also be realized in these platforms. Using comprehensive exact diagonalization calculations on twisted bilayer $MoTe_2$ at nu = -4/3 and an idealized Landau level model, we conjecture that FTIs can be obtained under realistic conditions, and extract general principles for engineering such exotic phases. Our analysis accounts for microscopic details such as band-mixing and anisotropic non-local dielectric screening.

14:45 | **127**

Ferromagnetic quantum critical point protected by nonsymmorphic symmetry in a dense Kondo metal $CeSi_{1.97}$

Soohyeon Shin, Aline Ramires, Vladimir Pomjakushin, Igor Plokhikh, Ekaterina Pomjakushina,
Paul Scherrer Institut

Quantum critical points (QCPs) are windows to fundamental quantum mechanical phenomena associated with universal behaviour. Recently, antisymmetric spin-orbit coupling in noncentrosymmetric systems was suggested to protect ferromagnetic QCPs. A dense Kondo lattice $CeSi_{2-}$, crystallising in a centrosymmetric structure, exhibits ferromagnetic order when Si is replaced with Ag. We report that the Ag-substitution to $CeSi_{1.97}$ linearly suppresses the ferromagnetic order towards a QCP, accompanied by concurrent strange-metal behaviour. Herein, we suggest that, despite the centrosymmetric structure, spin-orbit coupling arising from the local noncentrosymmetric structure, in combination with nonsymmorphic symmetry, can protect ferromagnetic QCPs. Our findings offer a general guideline for discovering new ferromagnetic QCPs.

15:00 | ***END***

ID | KOND Poster

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The three-dimensional multiferroic domain structure of hexagonal manganites

Aaron Merlin Müller, Manfred Fiebig, Lukas Heckendorn, Thomas Lottermoser, ETH Zürich

We simulate and visualize the three-dimensional domain structure of multiferroic hexagonal manganites using phase-field simulations. Due to the improper nature of their ferroelectric order, hexagonal manganites exhibit unconventional six-fold vortices in their ferroelectric domain patterns. In 3D, these domain patterns are characterized by vortex lines, which are 1D topological defects that form loops. Below the Néel temperature, an additional antiferromagnetic order rigidly coupled with the ferroelectric order emerges, forming vortex domain patterns of its own. In our simulations, we observe new types of antiferromagnetic three-fold, four-fold and six-fold vortex lines in addition to ferroelectric six-fold vortex lines. We relate the existence of these vortex lines to rigid coupling between orders.

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Identification of Defect-Sensitive Raman Modes in 9-Atom-Wide Armchair Graphene Nanoribbons

Ángel Labordet [1], Mickaël Lucien Perrin [1], Roman Fasel [1], Michel Calame [1,2], Gabriela Borin Barin [1],
Mirjana Dimitrievska [1]
[1] Empa, [2] University of Basel

Graphene nanoribbons (GNRs) are narrow strips of graphene with width-dependent electronic bandgaps, making them promising building blocks for nanoelectronic devices. However, structural defects can alter their electronic and optical properties, making defect characterization in GNRs a crucial step towards their further development. We use angle-resolved polarized Raman spectroscopy and density functional theory calculations to identify defect-sensitive Raman modes in 9-atom-wide armchair GNRs. Our results demonstrate that specific Raman peaks, namely the D and CH modes, exhibit distinct deviations from theoretically predicted angular dependence, serving as fingerprints for defect presence. These results provide valuable insights for non-destructive characterization of GNR quality and pave the way for defect engineering in GNR-based devices.

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Symmetry broken phases of field biased Bernal bilayer graphene

Enrique Aguilar-Mendez, Glenn Wagner, ETH Zürich

Using Hartree-Fock calculations we explored the possibility of spin,valley and translational symmetry breaking in Bernal bilayer graphene. Our aim is to explain the phases present near the van Hove singularity that arises in the band structure when an out-of-plane electric field is applied. A displacement field versus carrier density phase diagram was obtained in good agreement with experimental data. A slight tendency towards a valley coherence wave was found.