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Advancements in Genetic Design Automation Tools

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Description

Motivated by recent experimental progress we revisit the theory of pump–probe time- and angle-resolved photoemission spectroscopy (trARPES), which is one of the most powerful techniques to trace transient pump-driven modifications of the electronic properties. The pump-induced dynamics can be described in different gauges for the light–matter interaction. Standard minimal coupling leads to the velocity gauge, defined by linear coupling to the vector potential. In the context of tight-binding (TB) models, the Peierls substitution is the commonly employed scheme for single-band models. Multi-orbital extensions including the coupling of the dipole moments to the electric field – have been introduced and tested recently.

Time- and angular-resolved photoemission spectroscopy (trARPES) can directly probe the electronic structure of quantum materials out of equilibrium. This can shed light on the interaction of the electrons with spin, lattice, and orbital degrees of freedom, and help to unravel pathways towards novel out-of-equilibrium phases. Dynamical mean-field theory (DMFT) and its extensions provide a versatile toolbox to interpret such experiments through a theoretical simulation of the underlying microscopic processes. The approach can be applied both to Mott insulators and correlated metals, and it is formulated in terms of non-equilibrium Green's functions, which directly relate to the photoemission spectrum. This article reviews the theoretical description of trARPES within DMFT and related diagrammatic non-equilibrium Green's function techniques.

We investigated the effect of La substitutional ions on the structural, optical, and electrochemical properties of bismuth ferrite (BiFeO3) and used them as electrode materials for high performance supercapacitors. The compositions of 1.05Bi1-xLaxFeO3 (0.0 < x <0.10) nanoparticles were prepared through sol-gel conventional route and denoted as 1.05BiFeO3: BF0; 1.05Bi0.95La0.05FeO3: BF5; 1.05Bi0.90La0.10FeO3: BF10. The Rietveld refinement results of XRD patterns suggested the formation of rhombohedrally distorted perovskite structure (space group: R3c) with negligible secondary phase. The crystallite sizes determined using Scherrer's formula were found to be in the 59−48 nm range and observed to decrease with an increase in La content. The bandgap measured using UV absorption spectroscopy was found to decrease with an increase in La content in BiFeO3. The SEM micrographs revealed that the prepared samples were composed of nanocrystalline grains with particle sizes ranging from 25 to 40 nm. The electronic structural modification has been confirmed by the XAS analysis of Fe L3,2 and O K edge spectra as a result of La doping. Electrochemical measurements showed that 5% La-doped BFO (BF5) as an electrode demonstrated excellent performance for supercapacitors with a specific capacitance of 328 F g−1 measured with a scan rate of 10 mV s−1. It also exhibited tremendous cyclic stability with capacitance retention of >97 % for 1000 cycles measured at 1A g−1. Several applications are discussed, including the photo-induced melting of excitonic order, femtosecond relaxation processes in Mott insulators, and the manipulation of the electronic structure of Mott and charge transfer insulators using photo-doping and strong THz fields. In this work, we derive the theory of time-resolved photoemission within both gauges from the perspective of nonequilibrium Green's functions. This approach naturally incorporates the photoelectron continuum, which allows for a direct calculation of the observable photocurrent. Following this route we introduce gauge-invariant expressions for the time-resolved photoemission signal. The theory is applied to graphene pumped with short terahertz pulses, which we treat within a first-principles TB model. We investigate the gauge invariance and discuss typical effects observed in subcycle time-resolved photoemission.

Scanning Electron Microscopy

Our formalism is an ideal starting point for realistic trARPES simulations including scattering effects. Using time-resolved multi-dimensional angle-resolved photoelectron spectroscopy (ARPES) we explore the angular momentum transfer of low energy polarized photons to two prototype topological insulators, BiTeSe

and BiSe. Our comparative study is based on the analysis of circular dichroism in the photoemission yield of photoexcited Dirac states, and reveals that the spin vector of in-gap Dirac electrons in BiTeSe presents a more pronounced out-of-plane component compared to that of BiSe. We show that the multi-dimensional ARPES approach can be effectively used to observe the spin texture of photoexcited topological insulators, and to unambiguously disentangle experimental geometry and matrix element effects. This work presents a study of the structural properties on four representative kaolinite samples.

Scanning Electron Microscopy (SEM), X-ray Diffraction (XRD), Thermochemical Analyses (DTA/TGA), and X-ray Near Edge Structure (XANES) and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy measurements were carried out, and different empirical indices that quantify the structural order were assessed. Also, XRD patterns and EXAFS signals were compared to those corresponding to idealized defect-free structures calculated theoretically, to analyze the effects related to the structural disorder on real samples. The structural order at different scales (crystallographic, superficial, and local) was comprehensively examined for the four samples, and correlations between the order indices were performed and discussed, including the Debye-Waller factor obtained from Si K-edge EXAFS measurements. The proposed methodology shows that EXAFS is a suitable complementary technique that can provide valuable information about the Si local environments in natural kaolinites.

Time-Resolved X-ray Spectroscopies

Time-resolved X-ray spectroscopies have the potential of unveiling ultrafast processes with chemical sensitivity, but their widespread application is still withheld by technical and experimental constraints on two levels: the count rate and the amount of signal to be measured. In this paper, we will give a brief overview of the available pulsed X-ray sources focusing in particular on those delivering photons with energies inside the water window (280–550 eV), thus allowing accessing the C1s, N1s and O1s core levels which are relevant for the characterization of thin organic films and small molecules adsorbed on surfaces. We will mainly discuss the photon fluxes delivered by such sources in relation to their repetition rates, and we will see how these factors affect time-resolved measurements. The main purpose of this work is to discuss the most crucial parameter to adjust in pump-probe spectroscopies: the excitation density, which corresponds to the fraction of photoexcited molecules/atoms. We show that such quantity may be increased up to roughly 25% in gas phase and other robust samples, however, due to a lower damage threshold, in organic films it is typically constrained to be in the order of 1–5%. Despite the initially limited population of excited states in the latter case, we show that the evolution of the system may lead to a collective response of the material, which entirely modifies the measured core level line shape, thus providing a clear signal that may nonetheless offer valuable insights into the dynamics of the studied process.