

S06-CMPSP-208 / Poster presentation

Effect of Yttrium Substitution on Structural Properties of nanopowder nickel ferrites: X-Ray and Raman studies

Authors: Stevan Jankov¹; Elvira Toth¹; Maja Stojanovic¹; Sonja Skuban¹; Željka Cvejić¹

¹ *University of Novi Sad, Faculty of Sciences, Department of Physics*

Presenter: S. Jankov (stevan.jankov@df.uns.ac.rs)

Among various ferrites, nanosized nickel ferrite is one of the most frequently employed materials for production of electronic materials due to a set of outstanding physical and chemical properties. Doping with various atoms is a common choice when it comes to the development of new materials with target properties. Rare-earth elements have been frequently used in different research areas in order to improve various physical and chemical properties of materials. Nanocrystalline ferrites with chemical formula $\text{NiFe}_{2-x}\text{Y}_x\text{O}_4$ ($x = 0.20, 0.30$) have been synthesized by the co-precipitation method and further annealed at $750\text{ }^\circ\text{C}$. The details of the synthesis are given in [1]. X-Ray diffraction analysis (XRD) were carried out using Rigaky MiniFlex 600 diffractometer. Raman spectra were collected using a Thermo Scientific DXR Raman Microscope at room temperature with DPSS (Diode Pumped Solid State) laser using $\lambda = 532.2\text{ nm}$ excitation. CCD camera has been used as detector.

Spinel ferrites crystallize in cubic spinel structure belonging to space group $O7h$ ($Fd3m$). The recorded XRD patterns have confirmed the formation of spinel ferrite phase in the samples. No peaks corresponding to any precursor/impurity were recorded in the patterns implying that the samples are single phase. With the substitution of Y^{3+} in NFO, the whole diffraction pattern is shifted towards lower 2θ angle, which is a signature of an increase in lattice parameter of the substituted samples.

Group theory predicts the five Raman active modes, i.e. $A_{1g} + E_g + 3T_{2g}$. The measured spectra have been fitted and it is deconvoluted into individual Lorentzian component in order to determine the peak position. The spectra consists of band around $\sim 450, \sim 560, \sim 640, \sim 680, \sim 695\text{ cm}^{-1}$. The modes at above 600 cm^{-1} are related to the T-site mode that reflects the local lattice strain effect in the tetrahedral sublattice. The Raman modes below than 600 cm^{-1} corresponds to the O-site mode reflecting the local lattice strain effect in octahedral sublattice.

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Alternating-Basis Quantum Monte Carlo Method for Strongly Correlated Electrons

Authors: Jaksa Vucicevic¹; Veljko Jankovic¹

¹ *Institute of Physics Belgrade, University of Belgrade, Serbia*

Presenter: V. Jankovic (veljko.jankovic@ipb.ac.rs)

Ultracold-atom simulators have provided important insights into charge and spin transport in the two-dimensional Hubbard model [1, 2]. However, theoretical tools to compute quantities directly measured in experiments, such as space- and time-resolved charge/spin densities following a quench of an external density-modulating field, are still scarce. Here, we devise the alternating-basis quantum Monte Carlo (ABQMC) method for interacting electrons on a lattice, which is uniquely suited to compute such quantities. Apart from out-of-equilibrium setups, the formalism is equally applicable in thermal equilibrium described by either canonical or grand-canonical ensemble. The method relies on the Suzuki–Trotter decomposition (STD) and owes flexibility to the representation of the kinetic and interaction terms in the many-body bases in which they are diagonal. We formulate a Monte Carlo update scheme that respects both the momentum and particle-number conservation laws, to restrict the configuration space. The sampling efficiency is further enhanced by ensuring that the ABQMC algorithm manifestly respects several symmetries of the Hubbard model [3, 4]. We find that the method’s performance is heavily plagued by the fermionic sign problem, whose extent is primarily related to the number of time-slices in the STD. Nevertheless, the ABQMC equation of state (density vs. chemical potential curve) computed on square-lattice clusters containing up to 48 sites agrees remarkably well with reference methods. We also discuss how the (real-time) dynamics of the survival probability of pure density-wave-like states on 4x4 clusters depends on the filling and the initial density pattern.

Acknowledgement: The authors acknowledge funding provided by the Institute of Physics Belgrade, through the grant by the Ministry of Education, Science, and Technological Development of the Republic of Serbia, as well as by the Science Fund of the Republic of Serbia, under the Key2SM project (PROMIS program, Grant No. 6066160).

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Magnetic Hyperthermia Potential of Colloidal Zinc-substituted Iron Oxide Nanoparticles and TiO₂@Zinc Ferrite Hybrids

Author: Nataša Jović Orsini¹

Co-authors: Mirjana M. Milić¹; Tijana Marić²; Danijela Danilović¹; Gerardo F. Goya³