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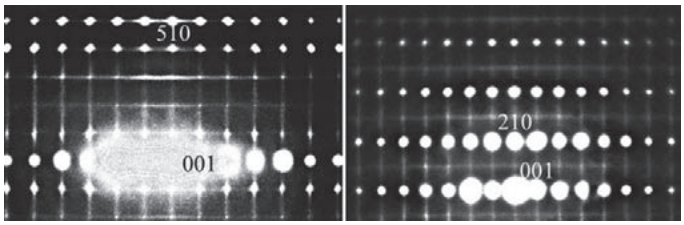
Structured diffuse scattering and polar nano-regions in $BaTiO_3$ doped relaxor ferroelectric systems

Ray L Withers[1], Yun Liu[1], Xiaoyong Wei[2], John D Fitz Gerald[3]
[1]The Australian National University, Research School of Chemistry, Building 35, Science Road, A.C.T, Canberra, A.C.T, 0200, Australia, [2]Electronic Materials Research Laboratory, Xian Jiaotong University, Xian, China, [3]Research School of Earth Sciences, Australian National University, Canberra, ACT, 0200, Australia., E-mail：withers@rsc.anu.edu.au

$BaTiO_3$-doped, relaxor ferroelectric systems exhibit broadened but still large peaks in dielectric permittivity as a function of temperature. The observation via electron diffraction of relatively sharp G+-{001}* sheets of diffuse intensity (see Fig.1) arising from the large amplitude excitation of 1-d inherently polar modes of distortion in such systems shows that the polar nano regions (PNRs) in these RF materials correspond to the same highly anisotropic <001> PNRs as are characteristic of the normal ferroelectric end member $BaTiO_3$ itself. The correlation length along the chains of these 1-D PNRs is estimated to be ~ 4-5 nm. The role of the dopant ions is not to directly induce PNRs but rather to set up random local strain fields preventing the condensation of long wavelength homogeneous strain distortion of the unit cell thereby suppressing transverse correlations of the inherent <001> chain dipoles and the development of long range ferroelectric order.



Keywords: relaxor ferroelectrics, diffuse diffraction, dielectrics

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Crystal structure and nonlinear optical behavior of N-(2 or 3-nitrobenzalidene)2,4-dimethylaniline

Ayhan Elmali[1], Asli; Karakas[2], Huseyin Unver[3]
[1]Ankara University, Faculty of Engineering, Engineering Physics, Ankara University, Faculty of Engineering, Department of Engineering Physics, Ankara, Beseveler, 06100, Turkey, [2]Department of Physics, Faculty of Arts and Sciences, Selcuk University, 42049 Campus, Konya, Turkey, [3]Department of Physics, Faculty of Sciences, Ankara University, Tandogan, 06100 Ankara, Turkey, E-mail：elmali@eng.ankara.edu.tr

N-(2-nitrobenzalidene)2,4-dimethylaniline (**1**) and N-(3-nitrobenzalidene)2,4-dimethylaniline (**2**) have been synthesized for the studies of their third-order optical nonlinearities. The structural characterizations have been determined by X-ray diffraction measurements. The maximum one-photon absorption (OPA) wavelengths evaluated theoretically using the configuration interaction (CI) method are shorter than 450 nm, giving rise to good optical transparency in the visible and near IR regions. To test the microscopic third-order nonlinear optical (NLO) behavior, linear and second (hyper)polarizabilities of the studied compounds may be considered rather adequate. We have computed both dispersion-free (static) and also frequency-dependent (dynamic) linear polarizabilities and second hyperpolarizabilities at 825-1125 nm and 1050-1600 nm wavelength areas using time-dependent Hartree-Fock (TDHF) method. The *ab-initio* calculation results with non-zero values on (hyper)polarizabilities indicate that the synthesized molecules might possess microscopic third-order NLO phenomena.

Keywords: X-ray diffraction, third-order nonlinear optics, time-dependent hartree-fock

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Crystal structure and nonlinear optical properties of n-(3-hydroxybenzalidene)4-bromoaniline

Huseyin Unver[1], Asli Karakas[2], Ayhan Elmali[3]
[1]Ankara University, Faculty of Science, Physics, Ankara University, Faculty of Sceince, Department of Physics, Ankara, Beseveler, 06100, Turkey, [2]Department of Physics, Faculty of Arts and Sciences, Selcuk University, 42049 Campus, Konya, Turkey, [3]Ankara University, Faculty of Engineering, Department of Engineering Physics, Ankara, Beseveler, 06100, Turkey, E-mail：unver@science.ankara.edu.tr

N-(3-hydroxybenzalidene)4-bromoaniline has been synthesized and characterized by X-ray diffraction analysis. To understand the relationship between structure-property and nonlinear optic (NLO) of the examined compound, our study has been extended to compute the one- photon absorption (OPA) wavelengths, linear and second (hyper)polarizabilities. We have calculated both dispersion-free (static) and also frequency-dependent (dynamic) linear polarizabilities and second hyperpolarizabilities at 825-1125 nm and 1050-1600 nm wavelength areas using time-dependent Hartree-Fock (TDHF) method. According to the calculation results obtained by means of configuration interaction (CI) method on the linear optical behavior, the maximum OPA wavelengths are estimated in the UV region to be shorter than 450 nm, showing good optical transparency to the visible light. The *ab-initio* calculated non-zero (hyper)polarizability values imply that the examined compound might possess microscopic third-order NLO behavior.

Keywords: crystal structure, nonlinear optics, second hyperpolarizability

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Virtual chemistry - The game we all play

David Brown
McMaster University, Brockhouse Institute for Materials Research, 1280 Main St. W., Hamilton, Ontario, L8S 4M1, Canada, E-mail：idbrown@mcmaster.ca

The only real things in chemistry are the nuclei and the electron density; everything else is virtual: orbitals, resonance, hybridization, ionic and covalent bonds, electronegativity, bond-order (-strength, -number, -valence, -energy), even bonds themselves, and for condensed matter, atoms are nothing more than concepts we impose on the nuclei and electron density in the hope of making sense of what we see there. None of these concepts arises naturally from the electron density and none of them has a unique definition. Some of these concepts are useful because they have predictive power, but others lead to more confusion than enlightenment. Manipulating these virtual concepts to interpret chemical structure is a game we