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An algorithm to compute the electro-elastic fields for layers of unrestricted anisotropy. <u>Konrad Bojar</u>,
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We present an algorithm to compute the Green's function and the coupled electro-elastostatic fields in a 2D piezoelectric layer of unrestricted anisotropy and containing a distribution of straight line defects. Currently only three types of boundary conditions for the layer are accepted by the algorithm: mechanically uncoupled boundaries, clamped boundaries, one boundary clamped and one boundary mechanically uncoupled. In addition, it is assumed that the layer is adjoined to dielectric subspaces of known dielectric permittivities. The algorithm presented computes the result using the inverse Fourier transform. It is well-known that the Fourier amplitudes of the Green's function and the corresponding electro-elastostatic fields for a single defect in a medium of any anisotropy class may contain essential singularities at $k=0$. For example, for clamped boundaries there are poles of order 1 for any symmetry class [1], for mixed boundary conditions there are no singularities irrespective of possible anisotropy [1], and for a layer of cubic symmetry with uncoupled boundaries there are poles of order 1, 2, and 3 [2]. Other boundary conditions have been investigated in [1], but the results obtained there contain some errors and cannot be implemented until the formulas are corrected. The poles mentioned above exclude direct application of simple quadratures or the IFFT (the inverse FFT).

The first step of the algorithm is to calculate constants c for all poles of the form $c/k^n,\ n=1,2,3$. Once all such constants are known, the singularities are removed from the amplitudes by a simple subtraction. The singular part of the solution which corresponds to the subtracted term does not need to be computed; it was shown in [2, 3] that although the Green's function diverges polynomially when $x \to \infty$ (far from the defects), the electro-elastostatic fields exhibit a regular behavior at infinity if and only if all forces and force moments are equilibrated.

The second step of the algorithm is to compute the IFFT of the remainder of the above subtraction. Given the desired precision, the appropriate sampling frequency is calculated using the analytical estimate of the Filon-type quadrature error [4]. The remainder is sampled at the chosen sampling frequency and fed into the IFFT function (e.g. from the FFTW library). The same procedure is applied for every defect of the layer and the final result is obtained by summing the partial solutions.

The proposed algorithm is a building block of a future modeling tool where continuum and discrete solutions are combined by means of the Teodosiu semi-discrete method [5]. Such a tool may appear powerful for designers of multilayered piezoelectric transducers, HFETs, and alike active elements. This tool will easily outperform the FEM and BEM methods in precision, resolution, and computation time.

[1] Nowacki, J.P.; Static and dynamic coupled fields in bodies with piezo-effects or polarization gradient, LNACM 26, Springer, 2006. [2] Bojar, K.; Green's function and electro-elastic fields in a 2D piezoelectric strip with straight line defects and free boundaries: Fourier approach for bodies of cubic symmetry. *Int. J. Sci. Eng.*, 2010, submitted. [3] Bojar, K.; Green's function and electro-elastic fields in a 2D piezoelectric strip with straight line defects and free boundaries: Fourier approach for bodies of unrestricted anisotropy. *Int. J. Sci. Eng.*, 2010, in preparation. [4] Petras, K.; Error estimates for Filon quadrature formulae. *BIT Num. Math.*, 1990. [5] Teodosiu, C.; Elastic models of crystal defects, Springer, 1982.

Keywords: anisotropic piezoelasticity, singularities, computer algorithm development

FA4-MS28-P02

DFT studies of 2-Methyl-6-[2-(trifluoromethyl) phenyl-iminomethyl]phenol: in gas phase and solvent media. <u>Ümit Ceyaln</u>, Hasan Tanak, Recep Tapramaz, *Department of Physics,Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.*
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Schiff bases are of interest because they are known to show photochromism and thermochromism in the solid state; this may involve reversible proton transfer from the hydroxyl-O atom to the imine-N atom. In general, O-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and keto-amine (or quinoid) forms. Depending on the tautomers, two types of intra-molecular hydrogen bonds are possible: O—H⋯N in benzenoid and N—H⋯O in quinoid tautomers. The H atom in title compound (I) is located on atom O1, thus the phenol-imine tautomer is favored over the keto-amine form, as indicated by the C2—O1 and C8—N1 bond lengths [1]. These values are in good agreement with the related compound [2]. The dihedral angle between the aromatic rings is 38.79 (5)º. The molecular structure is stabilized by an intramolecular O—H…N hydrogen bond, which generates an S(6) ring. In addition, there is an intramolecular short C—H…F contact [1].
The experimental geometry of 2-Methyl-6-[2(trifluoromethyl) phenyliminomethyl]phenol obtained from single-crystal X-ray diffraction [1] was compared with those obtained from DFT methot in gas phase. In order to evaluate the energetic and dipole moment behavior of the title compound in solvent, we carried out optimization calculations in the three kinds of solvent (chloroform, ethanol and water). The methodology used in this investigation is centered on Onsager's reaction field theory.

[1] H. Tanak, M.Yavuz, and O. Büyükgüngör, Acta Cryst., 2009, E65, o2949. [2] E. Temel, Ç. Albayrak, M. Odabaşoğlu, and O. Buyukgungor Acta Cryst., 2007, E63, o374.

Keywords: DFT, Schiff Base, Solvent media

FA4-MS28-P03

The molecular dipole moment of a non linear optical compound The 4,4 DiMethyl Cyano Biphenyl (DMACB) : Theoretical and X-ray diffraction study. <u>Abdelkader CHOUAIH</u>, Naima BOUBEGRA, Mokhtaria DRISSI & Fodil HAMZAOUI, *Laboratoire SEA2M – Facultés des Sciences & Technologies – University of . Mostaganem Algeria.*
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We present here results of comparative study of electron charge density distribution in the 4,4 dimethylamino-cyanobiphenyl (DMACB) compound from X-ray data experiment and theoretical investigation using Ab initio Hartree Fock (HF) and density functional theory (DFT) employing B3LYP/ B3PW91 exchange correlation levels of

theory. First the electron charge density distribution was obtained from high resolution X-ray experiment at low temperature using XD package [1]. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978) [2]. The study of the molecular electron charge density distribution reveals the nature of inter-molecular interactions including charge transfer [3]. Thereafter the results obtained were the subject of a comparison to those determined by theoretical calculation.

The agreement between the experimental and theoretical results such as: atomic net charge, molecular dipole moment, electrostatic potential and electron density was satisfactory. Table and figure below gives the molecular dipole obtained with different models and the orientation of the X-ray diffraction dipole moment in the molecule of DMACB, respectively.

Table: Magnitude of the molecular dipole moment

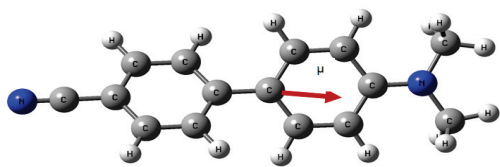| Models	X-ray diffraction	AM1	HF/6-31G**	DFT/B3LYP/6-31G**
μ (D)	5.80	5.1999	6.5974	8.4973

Figure: Orientation of dipole moment in DMACB

[1] Koritsanszky, T.; Howard, S.; Richter, T.; Su, Z.; Mallinson, P.R.; Hansen, N.K. XD a Computer Program Package, University of Berlin 2003. [2] Hansen & Coppens, Acta Cryst. (1978), A34, 909-921. [3] Coppens, P. X-ray Charge Densities and Chemical Bonding. New York: Oxford, 1997.

Keywords: Charge density, XD and Gaussian Software

FA4-MS28-P04

On the the use of single crystal diffractometer data necessary for performing the 2nd and 4th restricted moment method. Prabal Dasgupta, Bholanath Mondal
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With the advent of epoch-making paper by Groma & Borbely [1] &Borbely et al[2] renaissance of 2nd & 4th restricted moment method for evaluation of crystallite size has taken place..Above mentioned authors have reported that they have made use of high resolution XRD data .Present work aims to explore if the same technique may be applied to commonly used double crystal diffractometer data? To probe this,background & instrumental broadening corrected 111& 200 line of commercial gradeNi (in continous as well as in step-scan mode) were subjected to such analysis..M_2 & M_4/q^2 plots suggest that peak broadening in these materials are mainly crystallite size-related broadening. Different step-widths varying from0.005 to 0.03 and scan rate varying from 0.2 to 2.5 sec were chosen so as to ascertain the quality of data that yields more or less same crystallite size(within 5%) from the 2nd & 4th moment plot.It was revealed that XRD data

with stepwidth of 0.01deg or less and scan speed of at least 2.0 sec step $^{-1}$ in the step- scan mode as well as in continous mode yields satisfactory converegence.

[1] Borbely A. & Groma I.Appl. Phys.Lett.79 p-1772-1774,2001
[2] Borbely A., Revesz A. & Groma I.,Z.Krist.,Suppl,23,p-87,2006

Keywords: applied crystallography materials, powder method,crystallite size strain

FA4-MS28-P05

Theoretical and Crystallographic calculations on meta-Nitrophenol: a non linear optical compound.
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We investigated, in the present work, theoretically and experimentally the electron density distribution and electrostatic potential around the molecule m-Nitrophenol (m-NPH). The experimental determination and results of the molecule have been calculated from a high-resolution X-ray diffraction study. The X-ray experiment showed that there is an important accumulation of the electronic density around the connections of hydroxyl and nitro groups. Moreover, the lone pairs of the oxygen atoms were perfectly localized [1]. The x-ray data refinements were holed by using the XD software. XD uses the multipolar pseudo-atom model for the electron-density refinement [2]. The experimental charge density of the molecule m-NPH obtained by the multipolar model of Hansen and Coppens [3] is compared to the theoretical charge density determined from ab initio calculation. Theoretical calculations were performed with the Gaussian package at the density-functional (DFT) level of theory and semi empirical methods. The theoretical calculations carried out on the isolated molecule give results (net atomic charge, dipole moment, electrostatic potential …) in good agreement with those found in the experimental investigation.

Table below gives the molecular dipole moment in the inertial frame obtained with different models.

Table 1. Magnitude of the molecular dipole moment

Models	Multipolar refinement	AM1	MNDO	Ab initio
μ (D)	5.80	6.03	6.12	5.89

[1] Hamzaoui, F.; Baert, F.; Wojcik, G. Electron-density study of m-nitrophenol in the orthorhombic structure. Acta Cryst. B 1996, 52, 159-164. [2] Hansen & Coppens, Acta Cryst. (1978), A34, 909-921. [3] Hamzaoui F., Drissi M., Chouaih A., Vergoten G., International Journal of molecular Sciences, 2007, 8, 103-115

Keywords: charge density, XD Software

FA4-MS28-P06

PPDock-Portal Patch Dock: a web server for drug virtual screen and visualizing the docking structure by GP and X-Score. Po-Tsang Huang, Pei-Hua Lo, Chi-Hwa Wang, Chin-Tzong Pang, Kuo-Long Lou.
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