

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE NO.
1.1	Angular phase matching in a negative uniaxial crystal	7
1.2	Simple picture of the physical mechanisms of the nonlinearity of conjugated molecules. $ 0\rangle$ ground state, $ 1\rangle$ maximum charge transfer state and $ 2\rangle$ charge transfer from the acceptor to donor state (highly unlikely)	9
1.3	Typical example of engineering an organic molecule to obtain an acentric structure	11
1.4	The terahertz range of the electromagnetic spectrum	14
1.5	The effect of phase-mismatch and terahertz absorption on the effective generation length l_{gen}	19
1.6	Typical structure of a thin-film field-effect transistor	26
1.7	Typical current-voltage behavior for a p-type FET	27
1.8	Plot of the square root of source-drain current in the saturation regime as a function of the gate voltage. The line intercepts the VG-axis at the threshold voltage	29
1.9	Polycyclic aromatic hydrocarbons (PAHs)	31

FIGURE NO.	TITLE	PAGE NO.
1.10	Dependence of surface free energy, ΔG_s , volume energy, ΔG_v and change in free energy, ΔG , on the radius r of a homogeneous nucleus	33
1.11	Various positions of surface atoms in a crystal	34
1.12	Different stages of the formation of spiral from a screw dislocation	36
1.13	A typical solubility plot	37
2.1	Crystal growth chamber with Eurotherm temperature controller	44
2.2	Experimental setup for Kurtz powder technique	51
2.3	Experimental setup for Terahertz generation and detection	58
3.1	(a) ORTEP diagram (b) Optimized molecular structure of 2A4PNN	69
3.2	The molecular packing of 2A4PNN (a) In a unit cell (b) In the extended network, when projected along b axis (c) The herringbone structure of (010) plane of the unit cell (top layer of (010) plane alone is focused for clarity) (d) Schematic representation of herringbone structure	70
3.3	Solubility and Nucleation of 2A4PNN	79
3.4	As grown single crystals of 2A4PNN	80
3.5	BFDH Morphology of 2A4PNN	80

FIGURE NO.	TITLE	PAGE NO.
3.6	(a) Simulated and (b) experimental powder XRD patterns of 2A4PNN	81
3.7	FTIR spectrum of 2A4PNN	82
3.8	FT-Raman spectrum of 2A4PNN	82
3.9	(a) ¹ H NMR and (b) ¹³ C NMR spectrum of 2A4PNN	85
3.10	UV spectrum of 2A4PNN single crystal: (a) optical transmittance and (b) Tauc's plot (as inset)	86
3.11	(a) Emission and (b) Excitation spectrum of 2A4PNN single crystal	88
3.12	Particle size dependence of SHG output of 2A4PNN powder	90
3.13	TG/DTA curves of 2A4PNN crystalline powder	92
3.14	DSC curves of 2A4PNN crystalline powder	92
3.15	Temperature dependence of heat capacity of 2A4PNN	94
3.16	Micrograph of the laser-induced damage pattern of 2A4PNN single crystal	96
3.17	Temperature dependent (a) dielectric constant and (b) dielectric loss of 2A4PNN single crystal	99
3.18	(a) AC Current conductivity and (b) activation energy of 2A4PNN single crystal	102
3.19	Vickers Hardness indentation profile of 2A4PNN single crystal	104

FIGURE NO.	TITLE	PAGE NO.
3.20	Normalized transmittance as a function of Z position with (a) with open aperture and (b) with closed aperture	108
3.21	FMO analysis of 2A4PNN: (a) LUMO plot and (b) HOMO plot	113
3.22	(a) Mulliken charge analysis chart and (b) maximum atomic charges of 2A4PNN	114
4.1	Molecular structure of DAST material	119
4.1	High quality and twin-free DAST crystals by slow evaporation solution growth technique	119
4.2	Simulated and experimental powder XRD patterns of DAST	120
4.3(a)	Amplitude spectra of THz waves generated from DAST single crystals ordinate in the logarithmic scale	121
4.3(b)	Time-domain waveforms of the THz pulses obtained for the DAST single crystals of various solvents	122
4.5	Molecular structure of BNA material	123
4.4	Solubility of BNA material in polar protic and aprotic solvents	124
4.5	(a) BFDH Morphology of BNA; (b) & (c) Reported BNA single crystals (Notake et al. 2012; RIKEN, Japan)	124
4.6	(a) Simulated and experimental powder XRD patterns of BNA in (b) Ethyl acetate; (c) Acetonitrile; (d) dimethyl sulfoxide (DMSO);(e) DMSO : Acetonitrile (1 : 0.5); (f) Ethanol : Methanol (1 : 1); (g) Ethanol : Methanol : Acetonitrile (1 : 1 : 1)	126

FIGURE NO.	TITLE	PAGE NO.
4.7	Photographs of BNA single crystals (a) DMSO: Acetonitrile (1:0.5) (35 x 13 x 2 mm ³); (b) Ethanol: Methanol (1:1) (15 x 3 x 0.5 mm ³); (c) Acetonitrile + Ethanol+Methanol (1:1:1) (24 x 8 x 3 mm ³); (d) Ethyl acetate (8 x 4 x 3 mm ³); (e) Acetonitrile (11 x 7 x 4 mm ³); (f) DMSO (8 x 7 x 3 mm ³)	130
4.8	Schematic representation of desolvation and the rate of growth of various surface layers of BNA single crystal	131
4.9	Transmission spectrum of BNA single crystal in various solvents	135
4.10	X-Ray rocking curve (XRC) analysis of BNA single crystal (a) ethanol: methanol: acetonitrile (1:1:1); (b) acetonitrile; (c) ethyl acetate; (d) ethanol: methanol (1:1) and (e) DMSO	136
4.11	(a) Amplitude spectra of THz waves generated from BNA single crystals of various solvents with the ordinate in the logarithmic scale (b) Time-domain waveforms of the THz pulses obtained for the BNA single crystals of various solvents	139
4.12	Terahertz pulse characteristics (a) temporal evolution of the electric field, and (b) amplitude spectrum of the generated THz pulse	140

FIGURE NO.	TITLE	PAGE NO.
4.13	Pump-to-THz conversion efficiency. (a) Generated THz energy and (b) efficiency versus the pump fluence for laser pulse duration of 52 fs FWHM. (c) Spectral shift of the 800 nm pump when the THz is applied	142
4.14	Dependence of the generated THz pulse energy on the pump pulse temporal and spectral parameters. (a) Dependence of the THz output energy on the pump pulse duration for a wavelength of 820 nm. (b) Variation of the pump spectrum and (c) the corresponding change in the generation efficiency	144
5.1	Temperature program for rapid solution technique	151
5.2	Anthracene single crystals grown using various solvents: a) Carbon tetrachloride b) n-Hexane c) Carbon disulfide d) Xylene e) Chloroform.	152
5.3	As grown AN single crystal by rapid growth technique.	153
5.4	Digital photograph of thin and mechanically flexible AN single crystal.	153
5.5	Digital photographs of AN single crystal deposition on flexible substrate at different stage along with the schematic representation of the substrate positions	154

FIGURE NO.	TITLE	PAGE NO.
5.6	XRD pattern of (001) plane of AN single crystal	155
5.7	AFM image of 5 x 5 mm ² area of AN single crystal	156
5.8	Schematic representation of AN based OFET	157
5.9	OFET device fabricated AN single crystal	158
5.10	I–V characteristics of AN based OFET (inset shows the ISD vs V _g at 303 K)	159