

Enhancement of Optical Transparency and Structural Integrity of DMP Chalcone Crystal under Acoustic Shock Wave Exposure

N. Madhavan¹, F. Irine Maria Bincy¹, Oviya Sekar¹, Ikhyun Kim^{2,*} and S.A. Martin Britto Dhas^{1,2,*}

¹Shock Wave Research Laboratory, Department of Physics, Abdul Kalam Research Center, Sacred Heart College, Tirupattur, affiliated to Thiruvalluvar University, Serkkadu, Tamil Nadu, 635 601, India

²Department of Mechanical Engineering, Keimyung University, Daegu 42601, Republic of South Korea

Abstract: The nonlinear optical (NLO) properties of organic crystals are susceptible to their molecular structure and stability under extreme conditions. Herein, the (2E)-2-(3,4-dimethoxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one (DMP) chalcone crystal was synthesized and grown by a slow evaporation method, and its structural and optical responses under acoustic shock wave exposures were systematically investigated. Although previous reports indicate that the present crystal is thermally stable only up to 187 °C, the present work demonstrated remarkable resilience by withstanding transient acoustic shock conditions of approximately 0.59 MPa and 520 K without any signs of structural degradation, thereby demonstrating impressive resilience. XRD analysis indicated that no new diffraction peaks appeared after the shock exposure, confirming excellent phase stability of the crystal, while the variation in diffraction intensities and crystallite size indicated dynamic recrystallization. The crystallite size increased from 19 nm to 25 nm, which is accompanied by a decrease in lattice strain, indicating improvement in crystallinity. Further, optical microscopy showed a sequential process of defect creation and healing, and the crystal surface smoothed after the fourth and fifth shocks, consistent with shock-induced recrystallization. UV-Vis spectroscopy revealed a significant increase in optical transmittance from 31.6% to 71.5% and a slight modulation of the optical band gap from 3.21 eV to 3.32 eV, reflecting improved molecular ordering and reduced defect density. Overall, the structure remains stable while the band gap is tuned under acoustic shock waves, demonstrating that optical properties can be effectively modulated without disrupting the crystalline framework. This highlights acoustic shock wave exposure as a promising route for developing robust optoelectronic materials capable of reliable performance under extreme conditions. The findings further suggest that the acoustic shock wave technique can be used to engineer the microstructure and optical response of organic NLO crystals such as DMP, thereby expanding their potential for high-performance photonic and optoelectronic applications.

Keywords: DMP, Functional materials, Optoelectronics, Thin-film compatible chalcones, Optical bandgap engineering.

INTRODUCTION

The fast and ongoing progress of photonic and optoelectronic technologies has substantially enhanced the global need for new, high-performance materials with superior nonlinear optical (NLO) characteristics. Nonlinear optics is one of the central and most rapidly advancing fields of modern optical science, constituting the very basis of several state-of-the-art applications like optical signal processing, ultrafast telecommunications, frequency conversion, optical data storage, and the rapidly developing area of optical computing [1]. In general, materials for nonlinear optical applications are expected to show a balance of properties, including high thermal and chemical stability, strong and efficient nonlinear responses, as well as excellent optical transparency within a wide wavelength range in order to operate effectively and reliably in practical optical systems. Although extensive research and design efforts have been made focusing on these critical criteria, achieving a material that simultaneously meets all these demanding requirements continues to pose a significant scientific and technological challenge.

Organic materials remain among the most sought-after candidates in the vast and evolving branch of optoelectronics because of their numerous desirable optical characteristics, which include large nonlinear coefficients, ultrafast response times, and exceptional resistance to optical damage [2-4].

Moreover, organic nonlinear optical materials are attracting growing interest because their strong third-order responses and tunable molecular structures make them valuable in several energy-related photonic applications. The fast and efficient nonlinear behavior of these materials supports energy-efficient photonic systems, while strong nonlinear absorption enables effective optical limiting, as is also illustrated in the case of donor/acceptor-substituted chalcones. Organic nonlinear optical chromophores contribute to solar-energy conversion through enhanced photon-management processes and can be incorporated into thin-film optical coatings for laser protection and other photonic functionalities.

Among the diverse range of organic materials studied to date, chalcone derivatives stand out prominently due to their structural flexibility, which allows easy molecular tuning to optimize donor-acceptor interactions and overall optical

*Address correspondence to this author at the Department of Mechanical Engineering, Keimyung University, Daegu 42601, Republic of South Korea; E-mail: kimih@kmu.ac.kr & martinbritto@shcpt.edu

performance. These compounds are renowned for a wide array of advantageous features, including efficient power conversion capabilities, strong chemical and thermal stability, high optical damage thresholds, and favourable phase-matching properties. Furthermore, chalcone derivatives possess excellent blue-light transmission, substantial nonlinear optical coefficients, and short transmission cutoff wavelengths. Such properties are due to their extended conjugated π -electron system with alternating double bonds, allowing for greater charge delocalization and an appropriate optical response [6, 7].

Chalcone-based compounds thus provide a very efficient, versatile, and adaptable synthetic approach for the design and production of materials with pronounced nonlinear optical activity. In such molecular frameworks, the two benzene rings can be systematically modified by introducing a wide variety of electron-donating or electron-withdrawing substituent groups, such as OCH_3 , SCH_3 , Cl, or Br, to promote an uneven distribution of electronic charge in both the ground and excited electronic states. This induced intramolecular charge asymmetry significantly enhances the overall nonlinear optical response of the material [8]. Chalcone crystals, organic nonlinear optical (NLO) crystals derived from aromatic carbon-based molecular systems, have been widely studied as important parts in modern photonic devices. In recent years, increasing interest has also been paid to exploring the third-order nonlinearity of azo-dye-doped polymeric materials due to their exceptionally high optical nonlinearity, which is combined with a broad spectral response and ultrafast temporal response characteristics. Such unique properties make these materials very appealing for advanced photonic applications such as optical switching, optical limiting (OL), modulation, and other nonlinear optical technologies [9]. Several recent researches have also established the effective deposition of chalcone derivatives as thin films for optoelectronic and energy-related applications, emphasizing their importance in functional material design and photonic device engineering [10-12].

With all these advantages and promising features, not all chalcone-based NLO crystals behave optimally under any desirable experimental or operational conditions. One representative example is the (2E)-2-(3,4-dimethoxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one (DMP) Organic Crystal, which exhibits good nonlinear optical behavior with impressive thermal aspects but suffers from certain drawbacks. For instance, its thermal stability stretches only up to around 187 °C, which further restricts its use in high-temperature or high-power optical applications.

The DMP crystal also shows reverse saturable absorption and self-defocusing [13], which is not desirable in optical devices requiring saturable absorption or self-focusing characteristics for better functionality.

Also, the response of DMP under extreme conditions needs to be studied for the real time applications. To date, no report has been made on the investigation of acoustic shock wave exposure on the DMP crystal. The investigation of DMP structural and optical responses under such dynamic loading is of prime importance, as it gives insight into the crystal's structural integrity, phase stability, and resistance to external perturbations. Interestingly, such shock-wave exposure not only probes the material's structural robustness but can also influence its optical transparency key parameter in nonlinear optical applications. Enhanced transparency upon shock treatment might therefore indicate a higher molecular ordering or reduction of defect-related scattering centers and thus points toward better light transmission and stability. These findings are important in establishing the practical reliability and operational durability of DMP under extreme conditions. Besides, they set a scientific basis for the design of next-generation organic nonlinear optical materials with superior transparency, enhanced thermal endurance, and higher environmental resilience.

EXPERIMENTAL PROCEDURE

DMP crystal was prepared by mixing an equimolar amount of α -tetralone and 3,4-dimethoxy benzaldehyde in the ethanol of 250ml conical flask and stirring the compound for about 1 hour. The 10% NaOH solution was added dropwise and stirred for about 1 hour. The above reaction was placed at room temperature for 1 day, and the ice cubes were dropped into the solution beaker gently. After 1 day at room temperature, a yellow precipitate formed in the beaker, and the solution was washed with distilled water to remove the traces of NaOH. The raw material was dried and prepared for the crystal growth. 10 ml of Acetone was taken in a beaker, and the raw material was added gently till the achievement of supersaturation. Then the solution was filtered and placed in the beaker for 23 days. The obtained seed crystal was recrystallized three times in acetone to attain good quality, as shown in Figure 1. The size of the grown crystal has the dimensions of 10 X 8 X 3 mm³.

SHOCK WAVE LOADING TECHNIQUE ON DMP CRYSTAL

The grown DMP crystals were polished with emery sheets of grit sizes 3000 and 4000, being thinned to

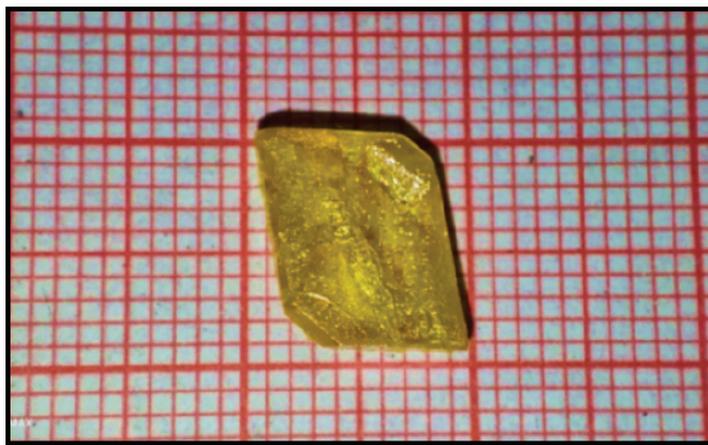


Figure 1: The photograph of an as-grown DMP crystal.

around 1 mm for shock loading studies. Shock waves were produced using a semi-automatic Reddy tube, which has three main sections: the driver, diaphragm, and driven sections. In this setup, an 80 GSM paper diaphragm acted as the rupture medium. The polished crystal sample was placed 1 cm from the open end of the driver section in a sample holder and exposed to one to five shock pulses. When the pressure in the driver section reached critical levels, the diaphragm ruptured, producing shock waves and propagating through the driven section and striking the sample placed in the sample holder. Each shock pulse's pressure was measured using piezoelectric PCB transducers (Model 113B26), which had a linearity error of 1% and a sensitivity of 1.465 mV/kPa. To ensure measurement accuracy, the transducers were calibrated under transient conditions of 0.59 MPa pressure and 520 K temperature, and their results were compared to standard reference data. The calibration results showed a standard error of less than 5%, indicating that the pressure readings are accurate and repeatable. The literature [14] has a comprehensive illustration of the semi-automatic Reddy tube arrangement. The structural and optical properties of the DMP crystal were then studied using powder X-ray diffraction (XRD), UV-Vis spectroscopy, and optical microscopy methods.

INSTRUMENTATION DETAILS

The DMP crystal's X-ray diffraction (XRD) patterns were acquired before and after shock loading using a Bruker D2 Phaser diffractometer. The diffraction data were taken across a 2θ range of 5° to 80° . The optical characteristics of the DMP crystal were investigated using a Varian Cary Bio 50 Spectrophotometer, with transmittance measurements taken in the 200-800 nm wavelength region. The crystal's surface morphology before and after shock exposure was investigated using an optical microscope (Weswox).

RESULTS AND DISCUSSION

X-Ray diffraction Analysis

Figure 2 shows the Molecular structure of the DMP crystal generated from CCDC ref:1968703. The title compound, (2E)-2-(3,4-Dimethoxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one, is a chalcone derivative with the molecular formula $C_{19}H_{18}O_3$. It consists of a 3,4-dimethoxyphenyl ring linked through an E-configured benzylidene double bond to a 3,4-dihydronaphthalen-1-one (tetralone) moiety. In the dihydronaphthalene system, the cyclohexanone ring adopts a distorted half-chair conformation, the atoms C9 and C10 deviating from the mean plane by -0.381 and $+0.285$ Å, respectively. The two aromatic rings are at a dihedral angle of 52.20° , indicating a moderate twist that reduces planarity, while both methoxy groups are nearly coplanar with their aromatic ring. In the crystal, the molecules are connected into zigzag C(12) chains by weak C-H \cdots O hydrogen bonds, while the overall packing is stabilized mainly by van der Waals interactions. The crystal of the title compound is orthorhombic, space group $P2_12_12_1$, with four molecules per unit cell ($Z = 4$). The unit cell parameters are $a = 7.9229$ Å, $b = 9.4474$ Å, $c = 20.875$ Å, while the cell volume is 1562.5 Å³. Such structural features are typical for the conjugated chalcone system and account for the potential of the title compound in optical and biological applications [15].

Figure 3 shows the XRD pattern of the DMP crystal (a) before and after exposure to shock waves (b) Zoomed version of (002), (112), and (212) planes. The obtained diffraction peaks are matched with CCDC ref:1968703 [15]. Upon subjecting the DMP crystal to shock pulse exposures, the diffraction pattern exhibited no emergence of new peaks or loss of existing ones, demonstrating its exceptional structural integrity and consistent crystalline phase. However, distinct variations were detected in the intensity of certain

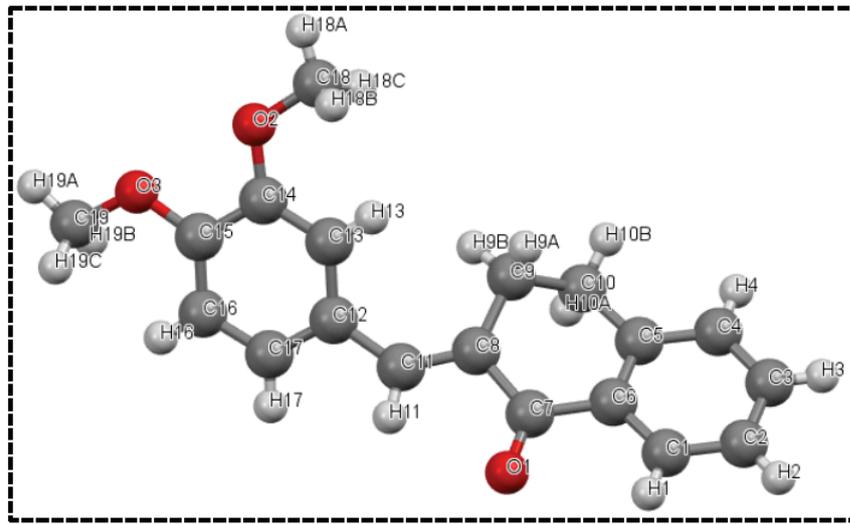


Figure 2: Molecular structure of DMP crystal generated from CCDC ref:1968703.

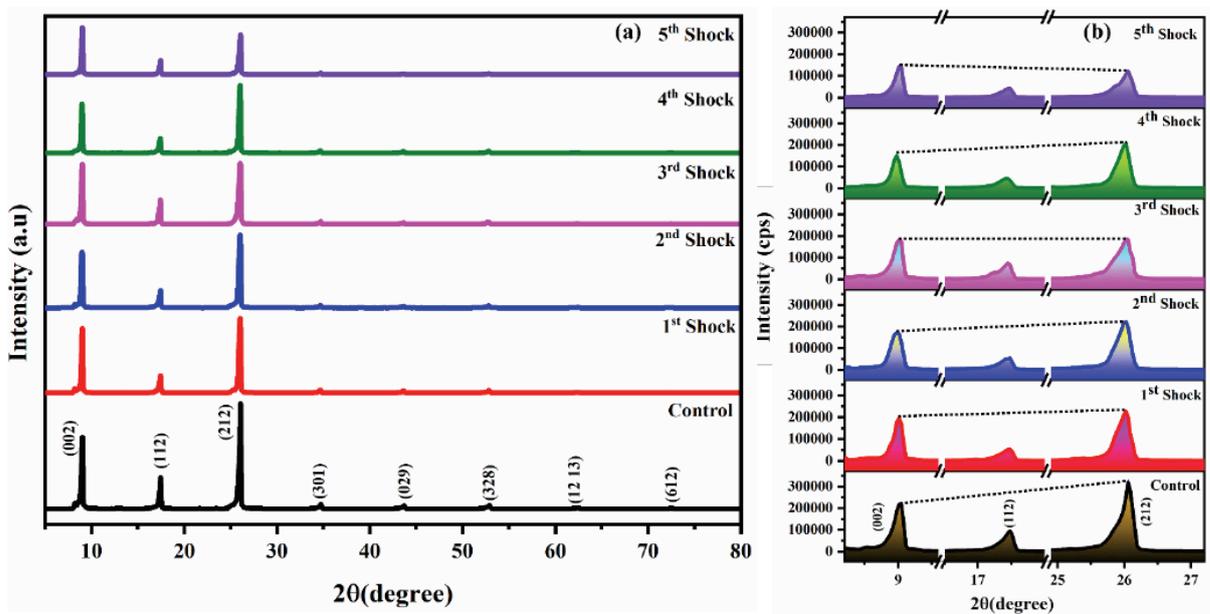


Figure 3: XRD pattern of DMP crystal (a) before and after exposure to shock waves (b) Zoomed version of (002), (112), and (212) planes.

diffraction planes, particularly in (002), (112), and (212) planes, indicating subtle changes in the crystal's internal alignment or strain distribution rather than any phase transformation. Such fluctuations result from rapid compression induced by shock waves, which leads to dynamic recrystallization and rearrangement of the crystal lattice. Therefore, the original crystal planes, particularly (002), (112), and (212), have partly rearranged, leading to significant changes in their intensities at the fifth shock pulses. This also shows an increase in the crystallinity of the DMP crystal upon repeated shock loading. As represented by its crystallography, the unit cell of the DMP shows anisotropic lattice behavior with some directions more compressible compared to other planes [16-18]. When the materials with anisotropic characteristics show

more substantial compressibility along the c-axis, which is elongated, compared to through the ab-plane, due to a difference in the strength of bonding and structural arrangement. In the DMP crystal, the bond along the elongated c-axis is held together by the weaker van der Waals forces, although other strong bonds dominate the ab-plane. These weak interlayer forces were more easily overcome under the compression caused by shock wave loading, leading to more significant compression along the c-axis due to its lower elastic modulus, or stiffness, compared to the ab-plane [19].

The average crystallite size of DMP crystals before and after shock loading was evaluated by using the Debye-Scherrer equation, $D = K\lambda/\beta\cos\theta$ [20]. The

lattice strain (ϵ) for the DMP crystal before and after shock loading was evaluated by using the following equation: $\epsilon = \beta / 4 \times \tan\theta$ [21]. Accordingly, the crystallite size of the unshocked DMP crystal was 19 nm, and after the shock wave exposure, it increased gradually to 20 nm after the first shock pulse, 21 nm after the second shock pulse, 22 nm after the third shock pulse, 23 nm after the fourth shock pulse, and 25 nm after the fifth shock pulse. This progressive increase in crystallite size is attributed to dynamic recrystallization prompted by shock waves. The high strain rates during each shock, along with the localized thermal effects produced, promote grain reorganization and refinement within the lattice structure, hence observable microstructural modifications [22]. Lattice strain, which reflects the density of lattice defects and the overall degree of crystallinity, is inversely related to crystallite size. As the crystallite size increases, the lattice strain correspondingly decreases. This occurs because larger crystallites have fewer grain boundaries and defects, resulting in reduced lattice imperfections and improved crystallinity. Consequently, the observed decline in lattice strain indicates a lower defect concentration and enhanced structural order in the DMP crystal [23, 24]. Figure 4 illustrates the relationship between crystallite size and lattice strain for DMP crystals before and after shock loading.

Optical Microscopic Analysis

Optical microscopy is a non-invasive, subjective technique for analyzing crystal surfaces. It enables the detection of morphological flaws such as fractures, pits, and voids, which have a substantial impact on a crystal's optical performance by acting as scattering and absorption sites for incident light. A series of optical micrographs, shown in Figure 5, was obtained of DMP crystals in their control state and after successive shock-wave exposures. The surface of the

control DMP crystal appears smooth, with faint, linear marks which may have resulted from slight scratches introduced during polishing with an emery sheet, indicating a minimum in surface imperfections and thus high crystalline quality. The application of the first shock wave induces a sharp but narrow diagonal feature that suggests the formation of a micro-crack or slip line associated with localized stress. The second shock wave reveals these lines, thus confirming the progressive development of defects as a result of repeated shock-loading. During the third shock, the pre-existing lines further widen and propagate, thus reflecting increased strain and fragmentation of crystal domains.

Interestingly, after the fourth shock pulses, noticeable smoothing occurs on the crystal surface. That is, the density and prominence of defects are considerably reduced. This trend is indicative of dynamic recrystallization impelled by transient high pressures and temperatures during shock events, thus leading to localized melting and rapid solidification that favors the rearrangement of molecules into a more orderly structure. Dynamic recrystallization requires $T > 0.4 T_m$, where T is the shock wave temperature and T_m is the melting point of the DMP crystal. The melting point of this crystal is stated to be 110 °C (383 K) [25-27]. Later, after the fifth shock, DMP crystals reveal a smoother surface, with further reduction in surface roughness. This suggests the onset of recovery phenomena where the destruction of lattice defects is favored and recrystallization occurs. From this alternating pattern of defect introduction and healing, it is perceived that shock waves might be employed for the microstructural evolution of DMP crystals in a controlled and reversible way, with each shock event

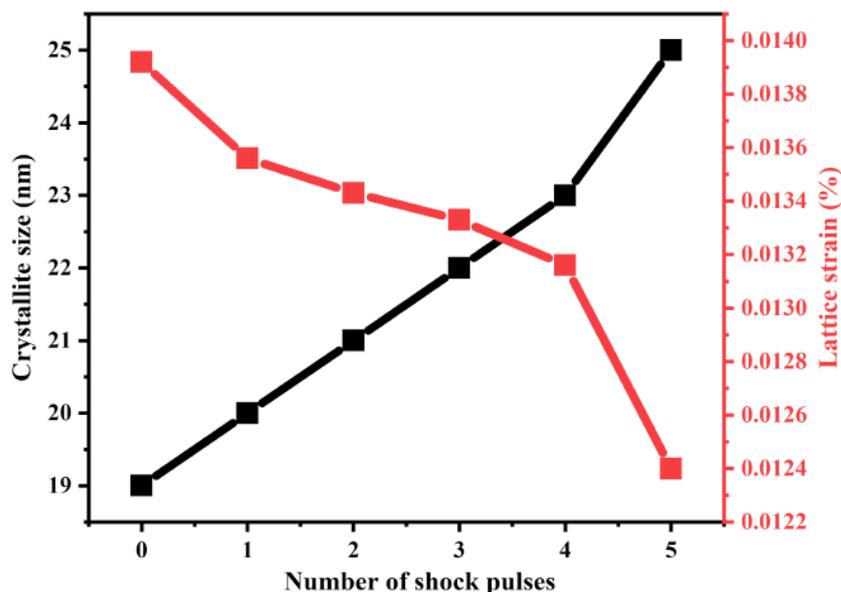


Figure 4: Variation plot of crystallite size vs lattice strain of DMP crystal before and after shock-loaded condition.

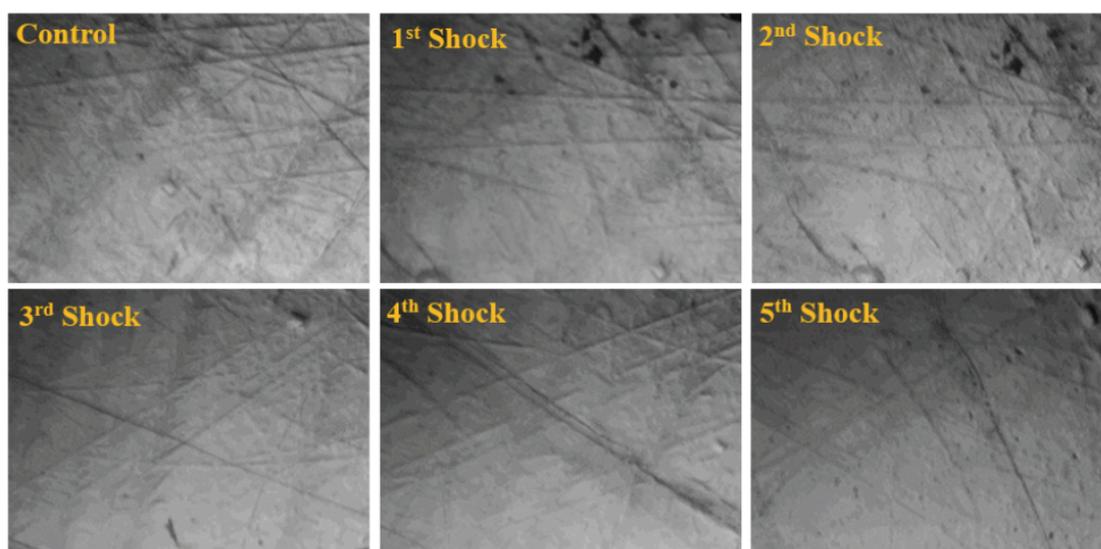


Figure 5: Optical microscopic image of DMP crystal before and after exposure to shock waves.

stimulating diffusion-driven rearrangement toward improved structural stability.

UV-Vis Analysis

The optical features of organic nonlinear optical (NLO) crystals, such as optical transmittance and the optical band gap, are critical metrics that determine their suitability for photonic and optoelectronic devices. Optical transmittance is extremely sensitive to the internal ordering of crystals, lattice strain, and the presence of structural defects; all of these can be strongly altered by dynamic loading such as shock pulses. To probe how successive shock pulses change the transparency of DMP crystals, we measured UV-Vis transmittance in the 200-800 nm shown in Figure 6 (a). The spectra show a clear absorption edge in the near-UV/blue region at 428 nm and a distinct increase in visible transmittance after shock treatment. Quantitatively, the unshocked (control) crystal exhibits moderate visible transmittance (31.6% at the reporting wavelength 800 nm), indicating low optical clarity for an organic NLO crystal.

After the first shock pulse, the measured transmittance increases substantially (to 54.4%), which we attribute to the rapid reorganization of surface and near-surface defects. The initial shock energy can relax localized lattice strain and remove or rearrange loosely bound impurities or trapped solvent molecules from growth sites, thereby reducing light-scattering centers and improving optical throughput. The second shock shows a reduction (45.2%) relative to the first-shock value, suggesting that the first pulse selectively healed some defects while the second pulse introduced a different distribution of microstrain or sub-surface disorder that temporarily increases scattering. With further shock exposure, the trend fluctuates but moves

to higher transparency overall: the third shock recovers to 53.9%, while the fourth and fifth shocks yield the highest transmittance values (67.4% and 71.5%, respectively). The progressive increase in transmittance percentage is shown in Figure 6 (b). This overall rise in transmittance with increasing shock number is consistent with gradual defect annealing and improvements in molecular packing and crystallinity. Shock energy can promote molecular layer reorientation, enhance π - π stacking, and reduce grain-boundary roughness that scatters visible light [28, 29].

The very large increases observed at the fourth and fifth pulses indicate a substantial reduction of internal scattering centres and improved optical homogeneity, implying stronger intermolecular interactions and more coherent domains within the crystal. To be sure, the non-monotonic fluctuation (rise \rightarrow dip \rightarrow rise) is significant: it shows that shock treatment can able to tune the crystals' transmittance. Early pulses can heal but also create different kinds of defects (e.g., relieve vacancy clusters but create local microstrain or dislocations), producing the observed fluctuation. As a result, the observed optical activity provides important information about the stability and potential for optoelectronic and photonic applications of DMP crystals, as well as a direct reflection of their substructural evolution under successive shock waves.

The optical band gap, determined via a Tauc analysis shown in Figure 7, is similarly sensitive to crystallite size, surface states, and defect chemistry. While the transmittance spectra here principally show changes in scattering and absorption background, modest shifts in the absorption edge and hence the extracted band gap are expected with changing crystallite size and defect population. The band gap of

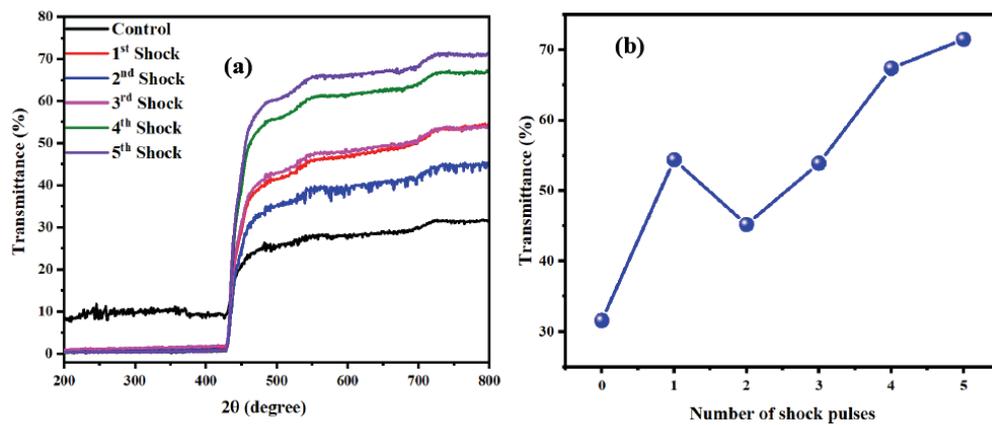


Figure 6: Transmittance graph and transmittance percentage of DMP crystal before and after exposure to shock waves.

the control DMP crystal is 3.21 eV, which is consistent with the literature [14]. For the shock-loaded samples, like the 1st shock, the band gap was increased to 3.31 eV, and then the band gap was dropped for the 2nd shocked conditions to 3.28 eV, and raised for the 3rd shock, 4th shock, and 5th shock to 3.29 eV, 3.31 eV, and 3.32 eV. In order to represent improved crystallinity and decreased mid-gap absorption, a decrease in defect states or an improvement in structural order tends to sharpen the absorption edge and raise the optical band gap. On the other hand, the creation of new defect levels, local disorder, or sub-band states can reduce the apparent band gap and widen the edge (creating Urbach tails). Defect reorganization and electronic-structure modification brought on by controlled shock loading are thus consistent with the observed changes, whether a widening or a narrowing of the band gap as well as the variations in transmittance and edge position [30-32]. This offers a flexible way to adjust the optical properties of DMP crystals for NLO applications. Most importantly, the structure remains stable while the band gap is tuned under acoustic shock waves, highlighting the potential to modulate optical properties without compromising crystalline integrity. In L-alaninium maleate (LAM) crystals, exposure to shock waves caused only minor surface defects and slight changes in optical transmittance, yet no structural phase transition occurred, confirming strong lattice resilience [33]. This indicates that acoustic shock waves can effectively fine-tune optical parameters such as transmittance and band gap while preserving the internal molecular framework. Such structural stability and optical tuning are highly relevant to the design of nonlinear optical and optoelectronic materials that can sustain high-pressure or high-temperature application environments for their operability in lasers, sensors, and advanced microelectronic devices that require both optical responsiveness and mechanical robustness. DMP's tunability and stability during shock exposure reveal its potential for future thin-film-based devices, despite the fact that the current tests use bulk crystals.

Chalcone derivatives are known for producing high-quality thin films, and the improvements in optical transparency, bandgap modulation, and crystallinity observed here directly support their use in photonic coatings, organic optical limiters, thin-film photodetectors, and energy-efficient optoelectronic layers. The defect-healing and recrystallization behavior under shock pulses suggests that pre-treated DMP may produce smoother, low-scattering films with better optical performance than untreated material, increasing its utility in thin-film technologies.

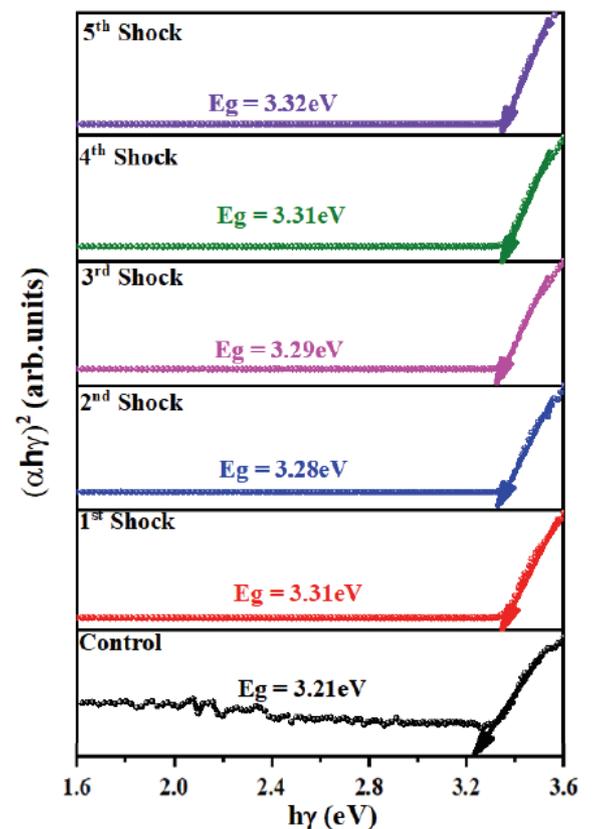


Figure 7: Tauc plot of DMP crystal before and after exposure to shock waves.

The interest in chalcone derivatives, such as DMP, for functional thin-film applications has been increasing

due to their π -conjugated backbone, high transparency, and tunable nonlinear optical response. Organic π -conjugated compounds are usually processed into thin films by means of various techniques, including spin-coating, drop-casting, thermal evaporation, and solution-assisted crystallization. Such methods may provide defect-controlled uniform films that are suitable for photonic coatings, flexible optoelectronic layers, and energy-efficient device platforms [34]. The shock wave-induced structural refinement, as evidenced in DMP, namely the enhancement of crystallite size, reduction in lattice strain, and improvement in optical transmittance, directly enhances its suitability for such film technologies [10]. Improved transparency and reduced defect density are particularly crucial in thin-film optical limiters, waveguides, photodetector coatings, and UV-visible window layers of energy-efficient photonic devices [35]. The acoustic shock processing enabled tunability of the optical bandgap (3.21-3.32 eV) that further indicates DMP can be engineered to meet specific spectral requirements during thin-film deposition. Therefore, the present results highlighted the fact that DMP is not only a robust bulk NLO crystal but also an excellent molecular candidate for next-generation functional thin films and energy-related photonic systems.

Shock-Wave-Induced Property Modulation in Bulk and Thin-Films

Defect engineering is a key method in functional thin films and energy materials, where lattice strain, dislocation density, and grain structure are regulated to modify optical, electrical, and photonic properties. Shock-wave-induced changes in DMP closely resemble such techniques. The dynamic recrystallization, strain relaxation, and defect annihilation caused by consecutive shock pulses resemble thermal annealing and strain-management procedures frequently utilized in thin-film production. These techniques result in sharper absorption edges, increased transparency, and tunable bandgap characteristics, all of which are important qualities for energy-efficient optoelectronic films. The current findings show that acoustic shock loading offers a low-energy alternative to traditional thermal or plasma-based post-processing methods. The ability to control the optical bandgap, reduce defect density, and promote crystallinity without modifying the molecular framework demonstrates shock-wave processing as a feasible approach for engineering organic materials before thin-film deposition. These findings link the behavior of bulk DMP under extreme conditions to defect-modulation protocols commonly used in thin-film and functional energy materials research.

CONCLUSION

The comprehensive investigation on the influence of acoustic shock wave exposure on (2E)-2-(3,4-dimethoxybenzylidene)-3,4-dihydronaphthalen-1(2H)-one crystals indicate their exceptional structural endurance and tunable optical behavior. Although the crystal of DMP has an intrinsic thermal stability limit of 187 °C, it maintained its stability under a shock wave of 0.59 MPa pressure and 520 K temperature without any structural decomposition or phase transition. Such exceptional resilience underlines the robustness of the chalcone-based molecular framework under extreme dynamic environments. X-ray diffraction results confirm that the orthorhombic lattice structure of DMP remains intact, while the progressive increase in crystallite size and the concurrent decrease in lattice strain indicate dynamic recrystallization and effective strain relaxation. Optical microscopy further corroborates these findings by revealing an evolution from defect initiation to subsequent defect healing and surface smoothing with repeated shock exposures, signifying the role of shock-induced thermal and mechanical effects in refining crystal morphology. The observed improvement in optical transmittance 31.6% in the unshocked state to 71.5% after five shocks-along with the marginal expansion of the optical band gap, from 3.21 to 3.32 eV, directly reflects a significant improvement in structural ordering and reduction of defect-mediated light scattering. The observed structural stability-optical tuning under acoustic shock waves confirms that optical properties can be engineered without compromising structural integrity. Such stability-driven tunability is vital for developing durable photonic and optoelectronic materials capable of sustained performance under extreme conditions. Acoustic shock wave treatment proves to be an effective technique for defect engineering, enhancement of crystallinity, and optimization of optical performance in organic nonlinear optical materials. The shock-wave-induced stability and tunability reported in this study make DMP a promising choice for thin-film photonic and energy-related applications. The improved transparency, lower defect density, and tunable bandgap make it suitable for use in optical coatings, photonic modulators, and energy-efficient optoelectronic devices. Furthermore, the findings suggest acoustic shock treatment as a promising defect-engineering strategy for preparing organic materials for future thin-film integration. Overall, DMP emerges as a structurally resilient and optically stable NLO crystal that retains its integrity under transient stress, offering new avenues to tailor the microstructural and optoelectronic properties of organic materials for advanced photonic, optoelectronic, and optical switching applications.

ACKNOWLEDGEMENT

The authors would like to thank the Abraham Panampara Research Fellowship (APRF). This research was supported by the Brain Pool program, funded through the National Research Foundation of Korea (RS-2023-00219593).

AUTHORS CONTRIBUTIONS

N. Madhavan- experiments, investigation, data analysis, and writing the original draft, F. Irine Maria Bincy- data analysis, and writing the original draft, S. Oviya- data analysis, and writing the original draft, Ikhyun Kim- analysis and resources, S. A. Martin Britto Dhas - conceptualization, investigation, writing, and editing.

DATA AND CODE AVAILABILITY

The data in this manuscript can be obtained from the corresponding author.

DECLARATIONS

Conflicts of Interest

The authors declare that they have no conflicts of interest regarding the publication of this paper.

Ethical Approval

None

REFERENCE

- [1] J. Badan, R. Hierle, A. Perigaud, J. Zyss, NLO properties of organic molecules and polymeric materials, in: D.J. Williams (Ed.), American Chemical Society Symposium Series, 233, American Chemical Society, Washington, DC, 1993.
- [2] D. Yu, D. Xue, *Acta Crystallographica B* 62 (2006) 702. <https://doi.org/10.1107/S0108768106018520>
- [3] R.L. Sutherland, *Handbook of Nonlinear Optics*, Dekker, New York, 1996.
- [4] D.S. Chemla, J. Zyss (Eds.), *Nonlinear Optical Properties of Organic Molecules and Crystals*, Academic Press, New York, 1997, vols. 1 and 2.
- [5] H.J. Ravindra, A. John Kiran, K. Chandrasekharan, H.D. Shashikala, S. M. dharmaprakash, Third order nonlinear optical properties and optical limiting in donor/acceptor substituted 4-methoxy chalcone derivatives. *Appl. Phys. B* 88, 105-110 (2007). <https://doi.org/10.1007/s00340-007-2677-8>
- [6] P.C. Rajesh Kumar, V. Ravindrachary, K. Janardhana, H.R. Manjunath, Prakash Karegouda, Vincent Crasta, M.A. Sridhar, *Journal of Molecular Structure* 1005 (2011) 1. <https://doi.org/10.1016/j.molstruc.2011.07.038>
- [7] D.N. Dhar, *The Chemistry of Chalcones and Related Compounds*, Wiley, New York, 1981.
- [8] R.A. Hann, D. Bloor, *Organic Materials for Non-linear Optics*, Royal Society of Chemistry, London, 1989, pp. 157.
- [9] A. Jawad Almosawe and H. L. Saadon, Nonlinear optical and optical limiting properties of new structures of organic nonlinear optical materials for photonic applications, *Chinese Optics Letters*, 11(4), 041902(2013). <https://doi.org/10.3788/COL201311.041902>
- [10] M. K. M. Ali, A. O. Elzupir, M. A. Ibrahim, I. I. Suliman, A. Modwi, H. Idriss, K. H. Ibrnaouf, Characterization of optical and morphological properties of chalcone thin films for optoelectronics applications. *Optik*, 145, pp.529-533, (2017). <https://doi.org/10.1016/j.ijleo.2017.08.044>
- [11] D. Haleshappa, S. N. Kakathkar, R. Bairy, M. S. Murari, The investigation of nonlinear optical response of chalcone and PMMA united thin films for photonic applications. *Materials Today: Proceedings*, 100, pp.31-36, (2024). <https://doi.org/10.1016/j.matpr.2023.04.476>
- [12] N. Syaharil, Synthesis, electrochemical analysis and DFT calculation of new alkoxyated-chalcone as semiconductor material, *Malaysian Journal of Analytical Sciences*, 26, (2022).
- [13] S. Nampoothiri, S. Chandran, S. Raj, R. Rajasekharan, N. Gummagol, L. Joseph, Third-Order Nonlinear Optical Studies of (2E)-2-(3,4-Dimethoxybenzylidene)-3,4-Dihydronaphthalen-1 (2H)-One Chalcone Derivative using Z-Scan Technique and DFT Method. *Crystal Research and Technology*, (2025), 60(8), p.e70011. <https://doi.org/10.1002/crat.70011>
- [14] F. Irine Maria Bincy, S. Oviya, P. Kannappan, Ikhyun Kim, S. A. Martin Britto Dhas. "Acoustic shock wave-driven dynamic recrystallization induced reversible rod-to-cube morphology transition in CdS: preserving structural integrity with optical modifications." *Dalton Transactions* (2025). <https://doi.org/10.1039/D5DT00998G>
- [15] D. Angeline Shirmila, D. Reuben Jonathan, M. Krishna Priya, J. Hemalatha, G. Usha, (2E)-2-(3,4-Dimethoxybenzylidene)-3,4-dihydronaphthalen-1 (2H)-one, *IUCr Data*, 2021, 6, x210309. <https://doi.org/10.1107/S2414314621003096>
- [16] V. Jayaram, A. Gupta, K. P. J. Reddy, Investigation of strong shock wave interactions with CeO₂ ceramic, *J. Adv. Ceram*, vol.3, pp.297-305, 2014. <https://doi.org/10.1007/s40145-014-0121-1>
- [17] I. Fedorov, D. Korabel nikov, C. Nguyen, A. Prosekov, Physicochemical properties of L-and DL-valine: first-principles calculations, *Amino Acids*, vol. 52, pp.425-433, 2020. <https://doi.org/10.1007/s00726-020-02818-3>
- [18] A. Sivakumar, S. Sahaya Jude Dhas, L. Dai, V. Mowlika, P. Sivaprakash, R. Suresh Kumar, A. I. Almansour, S. Arumugam, I. Kim, and S. A. Martin Britto Dhas, X-ray diffraction, and optical spectroscopic analysis on the crystallographic phase stability of shock wave loaded L-Valine, *J Mater Sci*, vol.58, pp.9210-9220, 2023. <https://doi.org/10.1007/s10853-023-08588-z>
- [19] J. Zhao, H. Liu, L. Ehm, D. Dong, Z. Chen, and G. Gu, High-pressure phase transitions, amorphization, and crystallization behaviors in Bi₂Se₃, *J. Phys.: Condens. Matter*, vol.25, pp.125602-125610, 2013. <https://doi.org/10.1088/0953-8984/25/12/125602>
- [20] S. Ravi, D. P. Bisen, S. U. Shukla, and B. G. Sharma, X-ray diffraction: a powerful method of characterizing nanomaterials, *Recent Research in Science and Technology* 4 (2012) 77-79.
- [21] M. Basak, M. L. Rahman, M. F. Ahmed, B. Biswas, and N. Sharmin, The use of X-ray diffraction peak profile analysis to determine the structural parameters of cobalt ferrite nanoparticles using Debye-Scherrer, Williamson-Hall, Halder-Wagner, and Size-strain plot: Different precipitating agent approach, *Journal of Alloys and Compounds* 895 (2022) 162694. <https://doi.org/10.1016/j.jallcom.2021.162694>
- [22] S. Ashok Kumar, S. S. R. Inbanathan, R. B. Vignesh, D. R. Rosaline, B. R. Kamalam, A. Uma, A. A. Ibrahim, S. Akbar, S. A. M. B. Dhas, and S. Baskoutas, Shock wave pulsed strategy on green synthesized nickel oxide nanoparticles: Structural, morphological, and electrochemical performance, *Ceramics International*, (2024), 51, 4509-4520. <https://doi.org/10.1016/j.ceramint.2024.11.426>
- [23] C.O. Ehi-Eromosele, B.I. Ita, and E.E.J. Iweala, Low-temperature combustion synthesis of cobalt magnesium ferrite magnetic nanoparticles effects of fuel-to-oxidizer ratio

- and sintering temperature, *J. Sol-Gel Sci. Technol.*, (2015), 76,298-308.
<https://doi.org/10.1007/s10971-015-3777-2>
- [24] B. Azhdar, Influence of fuel-to-oxidizer ratio, potential of hydrogen and annealing temperature on the structural and optical properties of nanocrystalline MgO powders synthesized by the hydrothermal method, *J. Exp. Nanosci.*, (2023), 18, 2276278-2276299.
<https://doi.org/10.1080/17458080.2023.2276278>
- [25] Y. I. Meshcheryakov, A. K. Divakov, S. A. Atroshenko, N. S. Naumova, Effect of velocity nonuniformity on the dynamic recrystallization of metals in shock waves. *Technical Physics Letters*, (2010), 36(12), pp.1125-1128.
<https://doi.org/10.1134/S1063785010120187>
- [26] S. Atroshenko, Metals dynamic recrystallization up to nanocrystalline size induced shock loading. In *AIP Conference Proceedings*, 2016, June, (Vol. 1748, No. 1, p. 030005). AIP Publishing LLC.
<https://doi.org/10.1063/1.4954351>
- [27] M. Deepa, S. Sahaya Jude Dhas, S. A. Martin Britto Dhas, Impact of shock waves on morphological, structural, optical and dielectric properties of l-alaninium maleate crystals. *Journal of Materials Research*, (2023), 38(18), pp.4303-4313.
<https://doi.org/10.1557/s43578-023-01143-1>
- [28] Deng, Ji-Hua, Jie Luo, Yue-Lei Mao, Shan Lai, Yun-Nan Gong, Di-Chang Zhong, and Tong-Bu Lu, π - π stacking interactions: Non-negligible forces for stabilizing porous supramolecular frameworks." *Science advances*, (2020), 6, no. 2, eaax9976.
<https://doi.org/10.1126/sciadv.aax9976>
- [29] A. V. Vologzhanina, Intermolecular interactions in functional crystalline materials: From data to knowledge. *Crystals*, (2019), 9 (9): 478.
<https://doi.org/10.3390/cryst9090478>
- [30] M. N. Siddique, T. Ali, A. Amed, and P. Tripathi, Enhanced electrical and thermal properties of pure and Ni substituted ZnO Nanoparticles, *Nano-Struct. Nano-Object.* (2018), vol. 16, pp. 156-166.
<https://doi.org/10.1016/j.nanoso.2018.06.001>
- [31] A. Ummadisingu, S. Meloni, A. Mattoni, W. Tress, M. Gratzel, Crystal-size-induced band gap tuning in perovskite films. *Angewandte Chemie International Edition*, (2021), 60(39), 21368-21376.
<https://doi.org/10.1002/anie.202106394>
- [32] S. Oviya, F. Irine Maria Bincy, Raju Suresh Kumar, P. Kannappan, Ikhyun Kim, S. A. Martin Britton Dhas, Reversible phase transition and tunable band gap in zinc telluride via acoustic shock. *Dalton Trans*, (2025) 54, pp.3188-3206.
<https://doi.org/10.1039/D4DT03393K>
- [33] M. Deepa, S. Sahaya Jude Dhas, S. A. Martin Britto Dhas, Impact of shock waves on morphological, structural, optical and dielectric properties of l-alaninium maleate crystals, *Journal of Materials Research*, 38, 4303-4313 (2023).
<https://doi.org/10.1557/s43578-023-01143-1>
- [34] R. A. Menezes, C. N. Bhuvaneshwari, H. Venkatachalam, K. S. Bhat, Focused review on applications of chalcone-based compounds in material science. *Discover Applied Sciences*, 7(8), p.814, (2025).
<https://doi.org/10.1007/s42452-025-07478-0>
- [35] P. Poornesh, S. Shettigar, G. Umesh, K. B. Manjunatha, K. P. Kamath, B. K. Sarojini, B. Narayana, Nonlinear optical studies on 1, 3-disubstituent chalcones doped polymer films. *Optical materials*, 31(6), pp.854-859, (2009).
<https://doi.org/10.1016/j.optmat.2008.09.007>

<https://doi.org/10.66000/3110-9772.2025.01.09>

© 2025 Madhavan *et al.*

This is an open-access article licensed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/4.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided the work is properly cited.