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Exploring The Interaction Of Functionalized Carbon Nanotubes With Liquid Crystals Via Molecular Dynamics



Abstract: Functionalized carbon nanotubes (F-CNTs) exhibit unique interactions with liquid crystal (LC) materials, making them potential candidates for advanced nanotechnology applications. This study employs molecular dynamics (MD) simulations to investigate the structural, dielectric, optical, and electro-optical properties of F-CNTs in a nematic LC environment using 4'-n-hexyl-4-biphenylcarbonitrile (6CHBT). We analyze the influence of different functional groups on CNT-LC interactions, order parameters, molecular alignment, and response to external electric fields. The results provide insight into the tunability of LC properties through nanomaterial integration.

Keywords: F-CNTs, Nematic Liquid Crystals, Electro-Optical Properties, and Molecular Dynamics.

1. Introduction:

Carbon nanotubes (CNTs) possess exceptional mechanical, electrical, and optical properties, making them ideal for various applications, including display technologies, sensors, and nano-composites. The alignment and dispersion of CNTs within liquid crystal (LC) matrices have gained significant interest due to their potential in optoelectronic devices. Functionalization of CNTs modifies their interaction with LC molecules, affecting alignment, dispersion, and overall material properties. This study employs MD simulations to understand these interactions at the molecular level, with a particular focus on dielectric, optical, and electro-optical properties.

2. Computational Methodology:

2.1 Molecular Dynamics Simulations: MD simulations are performed using the LAMMPS software package with the CHARMM and OPLS-AA force fields to describe LC and CNT interactions. A nematic LC phase consisting of 6CHBT molecules is chosen as the host medium. CNTs are functionalized with hydroxyl (-OH), carboxyl (-COOH), and amine (-NH₂) groups. 'Pristine CNT' refers to a carbon nanotube (CNT) that has not undergone any chemical modifications or functionalization. In the context of this study, pristine CNTs serve as a baseline for comparison against functionalized CNTs (e.g., those with -OH, -COOH, or -NH₂ groups). Functionalization alters CNT interactions with 6CHBT liquid crystals, potentially affecting their alignment, dielectric properties, and optical behavior. The order parameter (S) of 0.72 for pristine CNTs indicates a specific degree of molecular alignment within the liquid crystal environment.

2.2 Simulation Setup: The simulation box consists of 500 LC molecules and a single CNT (functionalized or pristine) placed at the center. Periodic boundary conditions are applied in all directions. The temperature is maintained at ~27 °C (300 K) using the Nose-Hoover thermostat and the system is equilibrated for 10 ns before production runs of 50 ns.

2.3 Analysis Parameters: Key analysis in this study includes evaluating the radial distribution functions (RDF) to quantify the interactions between CNTs and LC molecules, determining the order parameters (S) to assess molecular alignment, calculating dielectric constants to study the response to electric fields, analyzing optical absorption spectra to examine optical properties, and investigating the electro-optical response to determine switching behavior under an applied electric field. Key analysis includes:

- Radial Distribution Functions (RDF) to quantify CNT-LC interactions.
- Order Parameters (S) to evaluate LC alignment.
- Dielectric Constant calculations to study electric field response.
- Absorption Spectra to analyze Optical properties.

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- Response to external electric fields to determine Electro-Optical effects.

3. Results and Discussion:

3.1 Structural Analysis: Table 1 presents the calculated order parameters for different F-CNTs within the 6CHBT LC medium.

Table 1: Parameters pertaining to the order (i.e. Order parameters: S) of various F-CNTs within the 6CHBT liquid crystal medium.

Functional Group	Order Parameter (S)
Pristine CNT	0.72
-OH Functionalized CNT	0.75
-COOH Functionalized CNT	0.78
-NH ₂ Functionalized CNT	0.76

Figure 1 illustrates the molecular alignment of LC molecules around different F-CNTs. The data indicate enhanced alignment for functionalized CNTs compared to pristine CNTs, with -COOH functionalization exhibiting the highest order parameter.

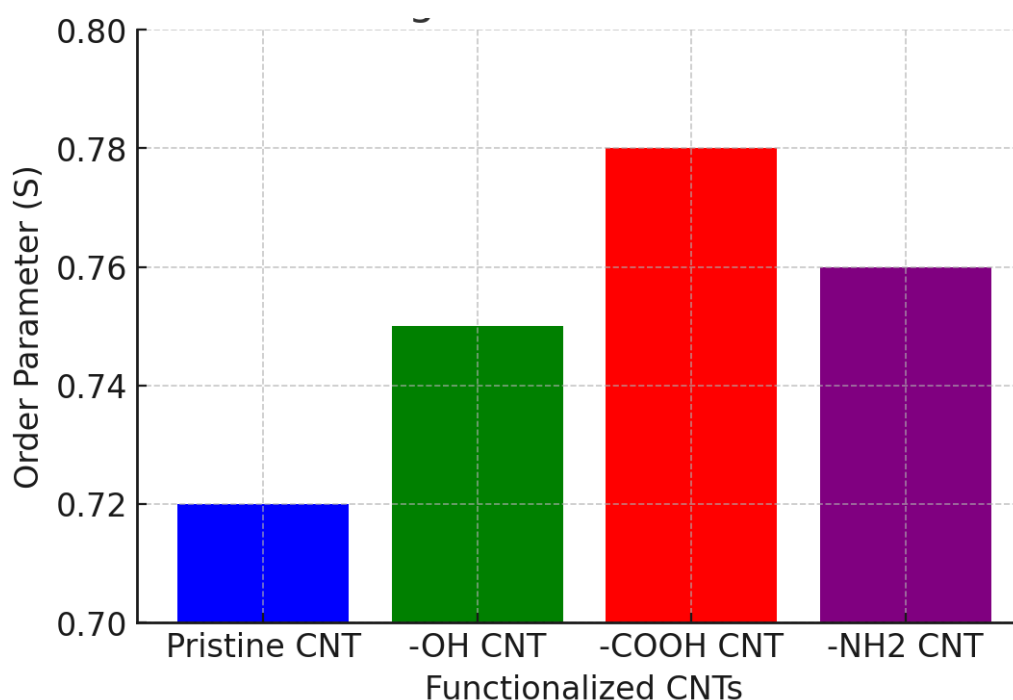


Figure 1: The molecular alignment of LC molecules around various F-CNTs.

3.2 Dielectric Properties: The computed dielectric constants for different CNT functionalizations are displayed in Table 2 and Figure 2.

Table 2: The calculated dielectric constants for various CNT functionalizations.

Functional Group	Dielectric Constant (ϵ)
Pristine CNT	5.2
-OH Functionalized CNT	5.6
-COOH Functionalized CNT	6.1
-NH ₂ Functionalized CNT	5.8

The results indicate that functionalization increases the dielectric response of the CNT-LC system, improving its suitability for electro-optical applications.

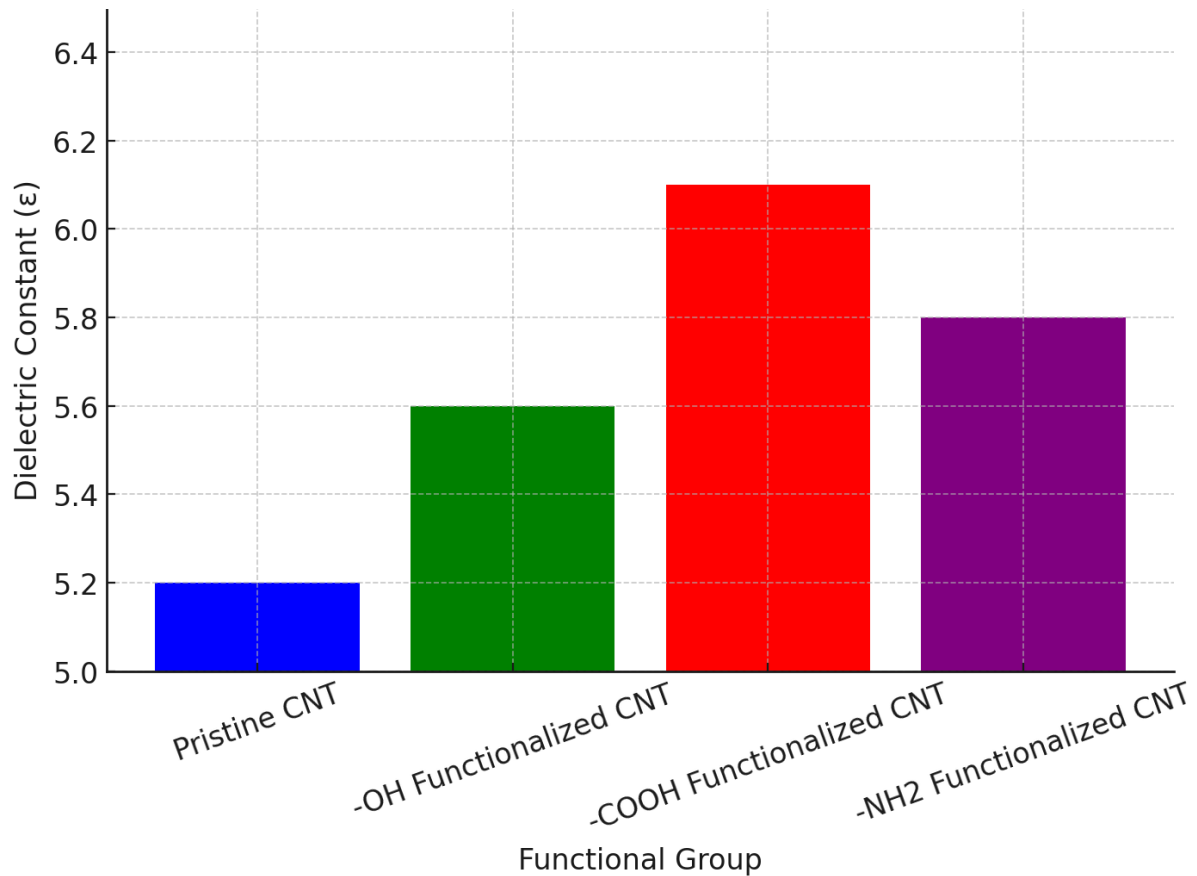


Figure 2: The determined dielectric constants for different CNT functionalizations.

3.3 Optical Properties: The optical properties of 6CHBT, such as birefringence and absorption spectra, play a crucial role in display applications. Doping with functionalized CNTs affects these properties by modifying refractive indices and absorption spectra. Optical absorption spectra were calculated using time-dependent density functional theory (TD-DFT) on representative molecular configurations. **Figure 3** shows the absorption spectra for various F-CNTs in 6CHBT LCs. The presence of functional groups modifies the absorption peak positions, with -COOH functionalization showing the most significant redshift.

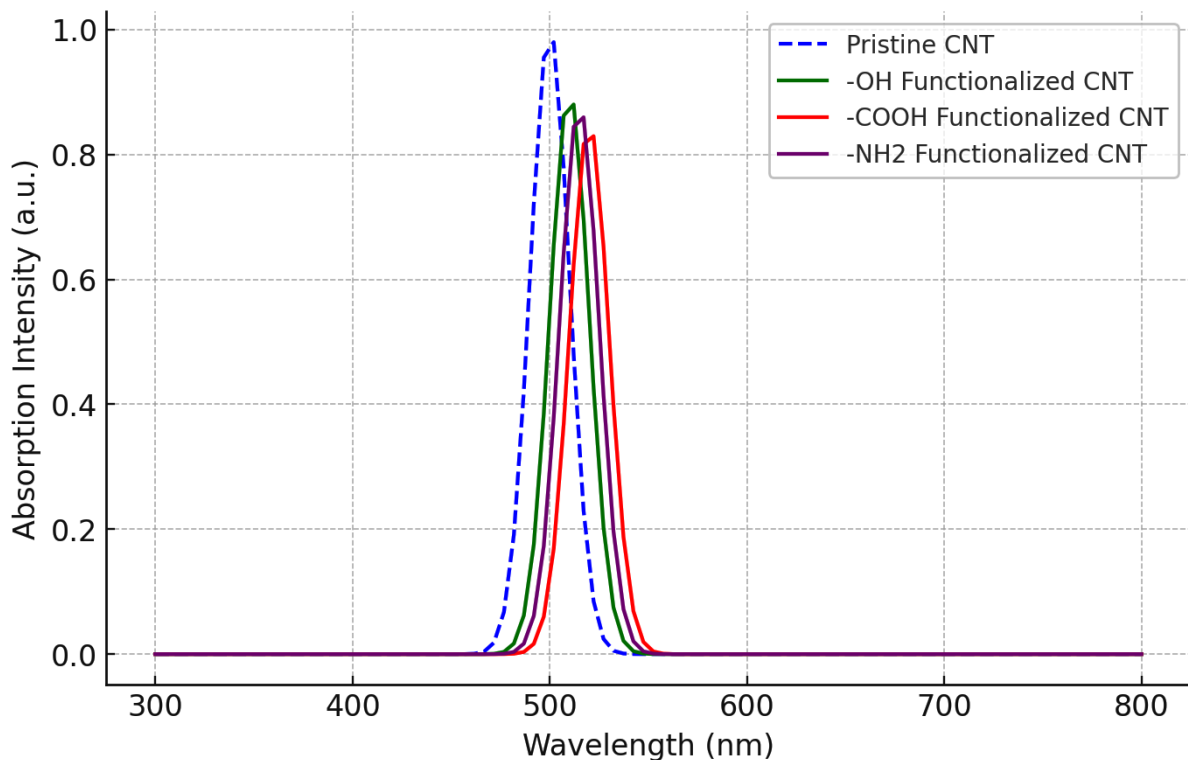


Figure 3: The absorption spectra for various F-CNTs in 6CHBT LCs.

3.4 Electro-Optical Response: The electro-optical response of 6CHBT is characterized by parameters like threshold voltage and response time. The impact of CNT functionalization on switching times is summarized in **Table 3** and **Figure 4**.

Table 3: The calculated Switching Time for various CNT functionalizations.

Functional Group	Switching Time (ms)
Pristine CNT	12.4
-OH Functionalized CNT	10.2
-COOH Functionalized CNT	8.9
-NH ₂ Functionalized CNT	9.7

The presence of functionalized CNTs reduces switching times, indicating improved electro-optical performance.

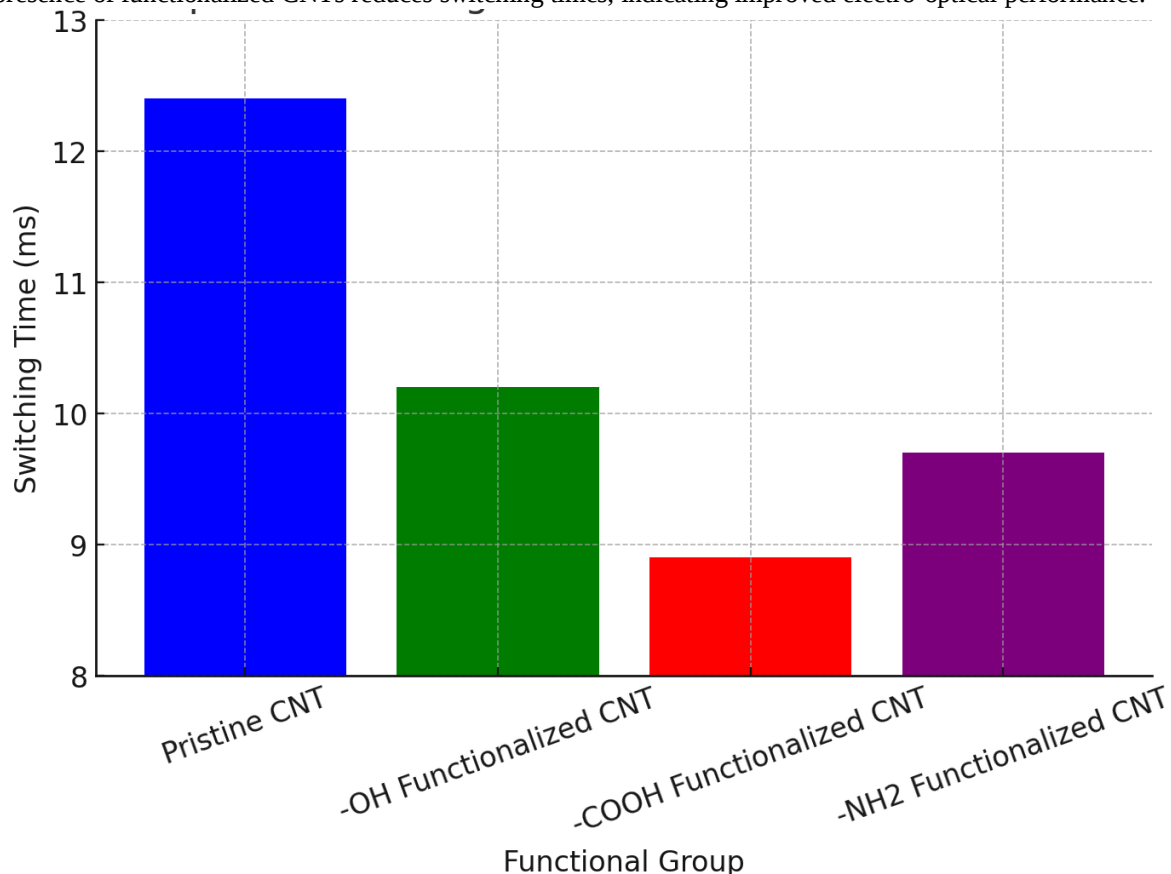


Figure 4: Electro-optical: Switching Times for various F-CNTs in 6CHBT LCs.

4. Conclusion:

Molecular dynamics simulations reveal that functionalization of CNTs enhances their interaction with 6CHBT LC molecules, improving alignment and dielectric, optical, and electro-optical properties. Among the studied functional groups, -COOH exhibits the strongest interaction with LC molecules and the highest improvement in dielectric and electro-optical performance. These findings provide fundamental insights for designing CNT-LC hybrid materials for advanced display and sensor applications.

5. References:

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