Spontaneous Orientation Polarization in TPBi Isomers: Insights into Structural Influence

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Spontaneous Orientation Polarization (SOP) arises from the partial alignment of molecular dipole moments (PDM) during vacuum deposition, creating a Giant Surface Potential (GSP) that significantly influences charge injection and transport in organic light-emitting diodes (OLEDs). Understanding the relationship between molecular structure and SOP behavior is critical for optimizing electron transport materials (ETMs). TPBi is a well known electron transporting material that shows SOP. Structural modification can modulate the degree of orientation by regulating the conformation.[1]

This study investigates SOP in TPBi and its three isomers (N1, N2, and N3) to explore how structural differences affect polarization performance. Kelvin probe measurements revealed distinct GSP slopes among the compounds. N1 exhibited the highest GSP slope (164.4 mV/nm), indicating strong polarization alignment, followed by N2 (122.8 mV/nm). N3, however, showed a negative slope (-37.0 mV/nm). These differences align with variations in PDM distributions and will be discussed using MD and DFT calculations.

The results emphasize the importance of molecular symmetry and dipole orientation in controlling SOP. While TPBi is a well-established ETM, the isomeric variations provide new insights into tailoring SOP through molecular design. This research highlights how structural modifications can systematically enhance charge transport and injection efficiency.

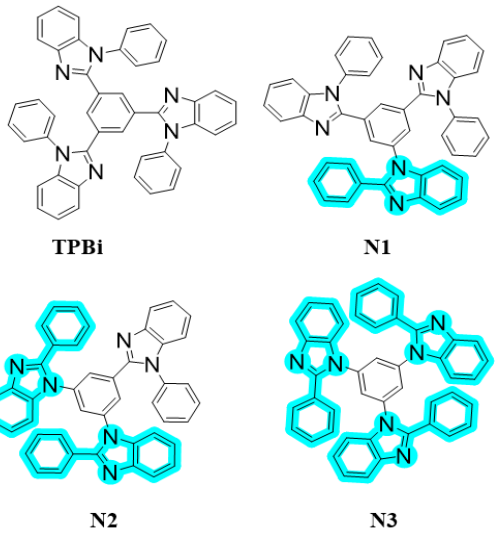

Fig. 1 Structure of TPBi and studied isomers.

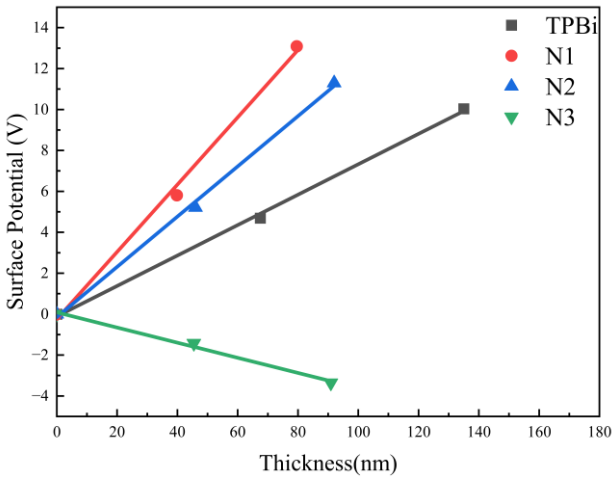

Fig. 2 Thickness dependence of surface potential for TPBi and its isomers.

Reference

1) W.-C. Wang, K. Nakano, D. Hashizume, C.-S. Hsu and K. Tajima, ACS Appl. Mater. Interfaces **14** , 18773 2022).