

# Nonradiative Transitions in Tetraphenylsiloles

Meghann E. Palmer,<sup>\*</sup> Murilo L. Tiago, Alex A. Demkov

*Physics Department, University of Texas at Austin, Austin, TX 78712*

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Tetraphenylsiloles (TPS) exhibit aggregation-enhanced photoluminescence, which is sensitive to the presence of nitroaromatic explosives such as trinitrotoluene (TNT). Detection of TNT therefore is possible by monitoring the luminescence signal [1]. To optimize the detection scheme it is important to understand the underlying electronic and structural interactions between the TPS and TNT molecules. These interactions can be studied using state-of-the-art theoretical methods thus aiding the design of potentially useful polymers. In particular, we consider 2,3,4,5-tetraphenylsiloles which have been shown experimentally to be only slightly luminescent as individual monomers in solution and highly luminescent when aggregated into oligomers [2]. Using density functional theory along with quasi-particle methods we investigate the electronic structure of the molecule and its luminescent properties. We consider the possibility that the relatively unhindered motion of the phenyl rings may provide a nonradiative transition channel.

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[1] S. J. Toal and W. C. Trogler, *J. Mater. Chem.* 16, 2871 (2006)

[2] J. Luo, et. al., *Chem. Communications*, 1740 (2001)

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<sup>\*</sup> *Email:* mepalmer@physics.utexas.edu