

Abstract Submitted
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Theoretical **Investigation**
of Nonradiative Transitions in Polysiloles¹ MEGHANN PALMER, MURILO
TIAGO, ALEX DEMKOV, The University of Texas at Austin — Silacyclopenta-
dienes, or siloles, exhibit aggregation-enhanced photoluminescence. Quenching of
luminescent nano-aggregates by electron deficient nitroaromatic explosives, such as
trinitrotoluene, may be monitored to detect explosives [1]. Detection relies on both
electronic and structural interactions between the sensing material and the ana-
lyte. These interactions can be studied using state-of-the-art theoretical methods
thus aiding the screening 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 aggre-
gated 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.

[1] H. Sohn, M. J. Sailor, D. Magde and W. C. Trogler, *J. Am. Chem. Soc.* **125**,
3821 (2003).

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

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