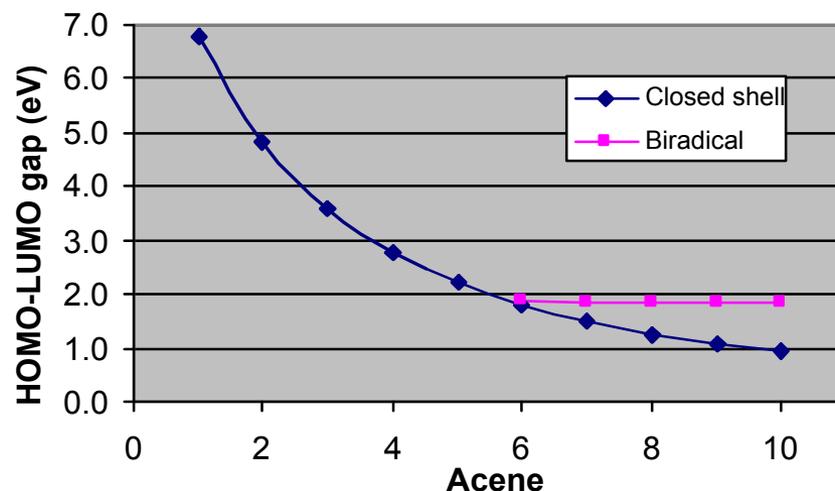


The Next Generation Organic Materials Oligoacenes, Heteroacenes and Cyclacenes

Fred Wudl, UCLA **DMR 0209651**

A series of oligoacenes from benzene to decacene were studied computationally using DFT and CASSCF methods. In contrast to the common view that acenes are closed-shell systems or may have a triplet ground state, these results offer the first theoretical prediction for the **singlet ground state and biradical character for oligoacenes**. The nature of the ground states of these molecules arises from the disjoint nature of the NBMOs occupied in the diradical.

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The blue line is based on restricted calculation forcing a closed shell. Extension to higher oligoacenes gives a meaningless lower than zero HOMO-LUMO gap. The pink line indicates an open shell singlet ground state.

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Education:

Under this grant, two students have completed their Ph.D. degrees: Dr. Xiangxu Chen and Dr. Hieu Duong and post-doctoral scientists have been trained: Dr. Kyle Starkey (GE) and Dr. Michael Bendikov (Weizman, Senior Lecturer), Dr. Dmitrii Perepichka (Senior Lecturer U. of Quebec); one REU undergraduate student has also been supported: Mr. Jeffrey Yamada and an undergraduate summer participant, Ms. Gizem Akcay . Currently, two Ph.D. graduate students: Mr. Ed Bolanos (4th year), Mr. Miguel Jimenez (2nd year), are also being supported.

Outreach:

Each summer, graduate students have participated in the summer high school teachers and student research programs, sponsored, in part by our NSF-IGERT, the Materials Creation and Training Program (MCTP).