# MINDING THE GAP – HIGHLY CORRELATED MULTIREFERENCE STUDIES OF AROMATIC POLYRADICALS

*Carol A. Parish*

Department of Chemistry, Gottwald Center for the Sciences, University of Richmond, Richmond, VA 23173, U.S.A.

The ability to characterize open-shell polyradical species and the cyclization reactions that involve such molecules holds significant promise for advancing the fields of multireference theoretical chemistry, mechanistic organic chemistry, materials design and drug optimization. This talk will describe our recent work using correlated multireference methods to characterize the low-lying electronic states of various aromatic and heteroaromatic polyradicals. In many cases, we find that these molecules possess a very high density of electronic states. For instance, in the naphthalene tetra-radical there are 5 states within 0.7 eV of the $^1A_g$ ground state, including a 2$^{nd}$ singlet, 3 triplets and a quintet. Polyradical geometries and energetic spacings provide insight into through-bond and through-space electron coupling and the role of aromaticity in the stability of these species.