

In honor of Bob Parr: Some thoughts on π systems and DFT

The stabilizing effect of a penalty function on the V state wave function of ethylene will be discussed. Some theorems about the use of a finite basis set in DFT will be presented. If time permits, our recent paper on benzene anion will be discussed. Also some unpublished work on molecular magnets will be discussed.

A systematic approach to the excited states of ethylene using configuration interaction and coupled cluster techniques. D. Feller, A. Peterson, E. R. Davidson, J. Chem. Phys. 141, 104302 (2014).

The benzene radical anion: a computationally demanding prototype for aromatic anion. A. P. Bazante, E. R. Davidson, and R. J. Bartlett, J. Chem. Phys. 142, 204304 (2015).