

## A EOM-CCSDT study of cationic small carbon rings

Yi-Fan Yang

*Quantum Theory Project, Departments of Chemistry, University of Florida, Gainesville,  
Florida, 32611*

The structure and properties of carbon ring system is a fascinating and challenging topic. Although the carbon rings have been found experimentally decades ago,<sup>[1]</sup> charactering properties of carbon rings correctly is still an ongoing challenge for both theoretical<sup>[2]</sup> and experimental researchers.<sup>[3]</sup> In this paper, we employed the state-of-the-art CCSDT and EOM-CCSDT methods to study the properties of small neutral and cationic carbon ring C<sub>6</sub> and C<sub>8</sub>. Surprisingly, we found that the EOM-CCSDT shows a different potential energy surface comparing to other CC methods, which results in different minimum and spectroscopy. The results indicate the necessary of introducing triple excitation of coupled-cluster method into the carbon ring system study.

### Reference:

[1] Prinzbach H, Weiler A, Landenberger P, et al. Gas-phase production and photoelectron spectroscopy of the smallest fullerene, C<sub>20</sub>[J]. *Nature*, 2000, 407(6800): 60-63.

[2] Brémond É, Pérez-Jiménez Á J, Adamo C, et al. sp-hybridized carbon allotrope molecular structures: An ongoing challenge for density-functional approximations[J]. *The Journal of Chemical Physics*, 2019, 151(21): 211104.

[3] Kaiser K, Scriven L M, Schulz F, et al. An sp-hybridized molecular carbon allotrope, cyclo [18] carbon[J]. *Science*, 2019, 365(6459): 1299-1301.