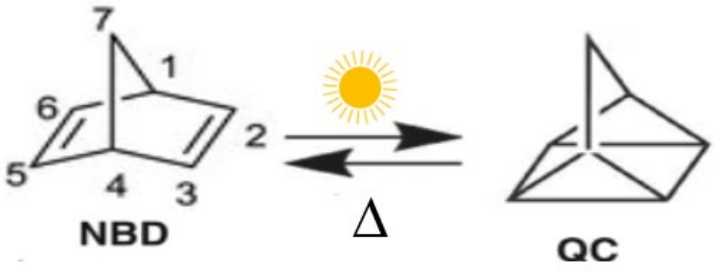
Storing the sunshine: outer valence ionization potentials of norbornadiene and quadricyclane

Feng Wang

Department of Chemistry and Biotechnology and Victorian Hydrogen Hub (VH2), Swinburne University of Technology, Melbourne, Victoria 3122, Australia

Hydrogen is considered as an inevitable green fuel of the future. Australia's National Hydrogen Strategy aims to position Australian industry as a major global player by 2030. A paradigm shift is needed towards clean energy under the current fossil fuel dominant energy consumption in the country. Hydrogen storage dominates the life cycle of hydrogen energy. Chemical storages dominate the major hydrogen storage techniques including liquid organic hydrogen carriers (LOHCs). The present study investigates the binary system of bicyclo[2.2.1]hepta-2,5-diene (norbornadiene) and quadricyclane photoswitches. In particular, the study will use the most recently measured ionic states of norbornadiene (NBD) and quadricyclane (QC) using synchrotron sourced radiation [1] in combination of an early (e,2e) measurement of Mackenzie-Ross et al [2] to theoretically study outer valence molecular orbitals in the isomerization. The through space interaction of NBD is confirmed as the next highest occupied molecular orbital ($10a_1$) od NDB.



[1] Palmer, M. H.; Coreno, M.; Simone, M. d.; Grazioli, C.; Aitken, R. A.; Hoffmann, S. V.; Jones, N. C.; Peureux, C., *The Journal of Chemical Physics* **2020,** *153* (20), 204303.

[2] Mackenzie-Ross, H.; Brunger, M. J.; Wang, F.; Adcock, W.; Maddern, T.; Campbell, L.; Newell, W. R.; McCarthy, I. E.; Weigold, E.; Appelbe, B.; Winkler, D. A. *The Journal of Physical Chemistry A* **2002,** *106* (41), 9573-9581.