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

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The study theoretically investigates outer valence molecular orbitals in the isomerization of of norbornadiene and quadricyclane. Through space interaction of NBD is confirmed as the next highest occupied molecular orbital (10a1) of NDB.

Primary author: WANG, Feng (Swinburne University of technology)Presenter: WANG, Feng (Swinburne University of technology)Session Classification: Poster session

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