

"Frustrated Carbon Pairs": from Stone Wales formation to astrocatalysis of H₂

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Using density functional theory (DFT), we studied the formation of Stone Wales defect in pyrene, as a PAH prototype, under interstellar conditions. We found that the formation of the defect requires overcoming two transition states of 8.26 eV and 8.42 eV and thus is unlikely to happen in space. However, the process might be catalyzed by an extra atomic hydrogen chemisorbed on the molecule. In addition, we studied the reactivity of "Frustrated Carbon Pairs" (FCPs) -- carbon pairs not directly bonded with each other due to the complete coordination and geometrical constraints -- in the pristine and defective pyrene throughout the hydrogenation processes that can occur in space. Our results suggest that FCPs are able to catalyze the extraction process that leads to the formation of molecular hydrogen under interstellar conditions.

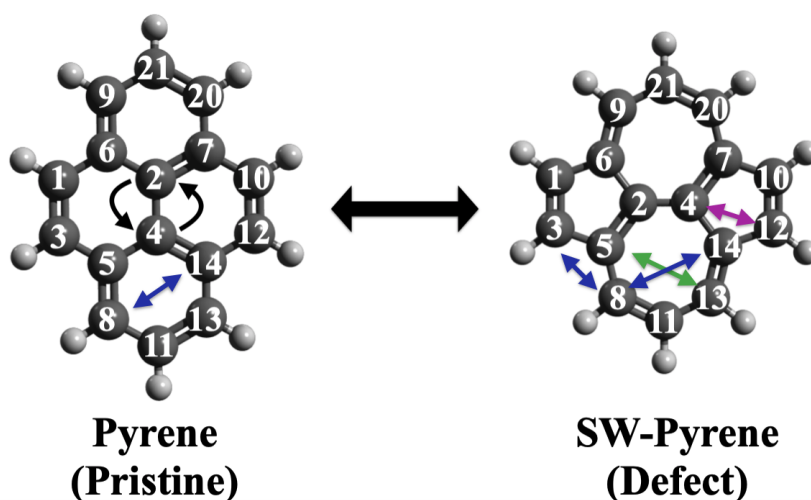


Figure 1: Schematic process of Stone Wales formation from pristine pyrene. Colored arrows show the FCPs studied in this work.

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