

## Theoretical study on the dissociation reactions of C<sub>4</sub>F<sub>6</sub> molecules

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Low-pressure fluorocarbon plasmas are widely used in microelectronics fabrication for a variety of surface modification purposes. In particular, fluorocarbon plasmas are used for the etching of dielectrics such as silicon dioxide and silicon nitride. Among the various fluorocarbons, this study focuses on C<sub>4</sub>F<sub>6</sub> molecules (C<sub>4</sub>F<sub>6</sub>s) which are composed of hexafluorocyclobutene (c-C<sub>4</sub>F<sub>6</sub>), hexafluoro-1,3-butadiene (1,3-C<sub>4</sub>F<sub>6</sub>), and hexafluoro-2-butyne (2-C<sub>4</sub>F<sub>6</sub>). We have investigated the dissociation reactions of C<sub>4</sub>F<sub>6</sub>s, resulting in CF<sub>2</sub>, CF<sub>3</sub>, C<sub>2</sub>F<sub>3</sub>, and C<sub>3</sub>F<sub>3</sub> fragments, by using the wB97X-D functional with various basis sets. In this presentation, the geometrical properties, energetics, and dissociation mechanisms of C<sub>4</sub>F<sub>6</sub>s will be suggested.