Abstract Submitted
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Computational Study on Dissociation Properties of C_4F_6 Molecules[1] HEECHOL CHOI, MI-YOUNG SONG, JUNG-SIK YOON, Plasma Technology Research Center, National Fusion Research Institute, PLASMA FUNDAMENTAL TECHNOLOGY RESEARCH TEAM — Saturated or unsaturated perfluorocarbons(PFCs) have been used extensively in dry etching processes due to their relatively low global warming potential and their high CF_2 radical levels in commercial plasma processes. Many experimental and theoretical studies of these species have been performed for useful information about physical and chemical properties of PFCs. Recently, it was reported that the ωB97X-D/aVTZ method is strongly recommended as the best practical density functional theory(DFT) for rigorous and extensive studies of PFCs because this theoretical level shows the high performance and reliability especially for van der Waals interactions. Among various PFCs, this study focuses on C_4F_6 molecules including c-C_4F_6, 1,3-C_4F_6, and 2-C_4F_6 isomers. All the feasible isomerization and dissociation paths of C_4F_6 molecules were investigated mainly at the ωB97X-D/aVTZ level. Their reaction rate constants were computed by using variational transition-state theory for a deep insight into C_4F_6's reaction mechanism. Fates and roles of C_4F_6 molecules and their fragments in plasma phases could be explained based on our theoretical results and data.

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