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Quantum chemical approaches toward searching for the low GWP plasma gas

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Saturated perfluorocarbons (PFCs) such as CF_4, C_2F_6, C_3F_8, and c-C_4F_8 conventionally used as dry-etch gases in the semiconductor industry have long atmosphere lifetimes and strong absorptions of infrared radiation, exhibiting high global warming potentials (GWPs) and so promoting the greenhouse effect[1]. Therefore, searching for the plasma gas with low GWP has been an important topic in the semiconductor industry for critical plasma etching processes together with global environmental protection. Theoretical structure, energetics, and kinetics data provide important information for experimental studies for the development of alternatives to conventional PFCs[2]. In this talk, we present quantum chemical approaches for the novel plasma gases. With the use of different levels of quantum chemical calculations, we show possible reaction pathways of plasma molecules and structures of reactants, products, and their transition states in an efficient manner. The energies and thermochemical properties of plasma molecules are obtained with high levels of quantum calculations. The reaction rates including the transition state theory (TST) and Rice–Ramsperger–Kassel–Marcus (RRKM) theory are also obtained for the stabilities of plasma molecules in various temperature and pressure conditions[3].

References

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