Theoretical Production of Physical and Chemical Data on Perfluorocarbons

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Many researchers in the fields of plasm modeling, plasma engineering, and plasma industry have tried to understand plasma gas chemistry and plasma-surface interactions such as chemical reactions, fregments, etch products, mechanisms, and so on. Actually, many experimental and theoretical studies have been performed for useful information on physical and chemical properties of plasma species. Unfortunately, it is very hard to get such data and information because plasma experiments are very sensitive to experimental conditions and high-level theoretical approaches need huge computational cost. Recently, we could conclude that the ωB97X-D/avtz method is strongly recommended as the best practical level of theory for rigorous and extensive studies especially of perfluoro carbon(PFC) plasma species [1]. Saturated and unsaturated PFCs have been used extentively in dry etching process due to their high CF_2 radical levels [2].

At the ωB97X-D/avtz level, structural, spectroscopic, energetic, and reaction properties as well as fundermental thermodynamic and orbital constants of PFCs such as electron affinity, ionization potential, polarizability, Lennard-Jones parameters, orbital energy, electron binding energy, etc were obtained. For a deep insight into some PFCs‘ reaction mechanisms, all the feasible chemical reaction paths were investigated at the same level of theory and reaction rate constants were computed by using transition-state theory [3]. Currently, these data are used in plasma modeling and diagnostics.

The theoretical methodology for physical and chemical data on PFCs and data production precesses will be shown in this ICAMDATA 2016 conference.

References

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