The Role of Density Functional Theory in Plasma Diagnostics and Simulations

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Many people in the fields of plasm modeling, plasma engineering, and plasma industry want to understand plasma gas chemistry about dissociation, isomerization, and recombination reaction properties as well as plasma-surface reaction properties. So, lots of experimental and theoretical studies have been performed to explain physical and chemical properties of plasma species and to obtain fundamental data on plasma gas and surface chemistry. Unfortunately, since plasma experiments are very sensitive to experimental conditions and high-level theoretical approaches need huge computational cost, there is still very little data available in literature and even some available data do not have exact and complete information on plasma molecules of interest. Density Functional Theory (DFT) is strongly recommended in the respect of computational cost and efficiency. Especially, the combination of wB97X-D and avtz basis set is the best level of DFT for perfluorocarbons (PFCs) based on rigorous and extensive theoretical studies on C_4F_8. At this DFT level, we have been trying to obtain the information on geometry, energetic, and thermodynamic constants which are key parameters in plasma simulations. The data on chemical reaction paths and rate constants of PFCs have been produced to analyse experimental results of their plasma diagnostics. In this talk, it will be presented that DFT plays an important role in analysing data from plasma experiments and supporting plasma simulations.