SiC is a wide bandgap semiconductor with many attractive properties. It has attracted particular attentions in the areas of power and sensor devices as well as biomedical and biosensor applications. This is owing to its properties such as large bandgap, high breakdown electric field, high thermal conductivities and chemically robustness.

Growth of the active layer of SiC is commonly carried out homoepitaxially using chemical vapor deposition (CVD) technique. It is difficult however to in situ measure what is happening inside the chamber in real time during growth. For this, computer simulations become a useful complementary tool. On the macroscopic scale (reactor scale), computational fluid dynamic (CFD) is a powerful method which allows predictions of heat and mass flow distributions, the types and concentration profiles of gaseous molecules as well as the profiles of growth rates and doping. To this end, CFD requires detailed input of all aspects ranging from material properties in heat and mass transports to elementary chemical reactions occurring in the process. Despite being highly needed, material properties and kinetics information are usually incomplete or missing.

In this thesis, quantum chemical calculations have been used to explore underlying mechanisms in the SiC CVD process as well as provide the missing data in thermochemistry and kinetics. Firstly, thermochemical properties of gas phase species relevant to SiC CVD processes have been derived and shown to be reliable compared to the available experimental and/or theoretical data. Secondly, by combining ab initio methods with conventional transition state theory, kinetic parameters were calculated for the gas phase and surface reactions related to the process. The data in the study is beneficial for modeling SiC CVD, and also for the study of graphene and diamond as well as fundamental studies.
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