PPDO 060

Computational Studies of Impurity Related Reactions During Gallium Arsenide Production

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Abstract

Arsine (AsH3) and trimethyl gallium (Ga(CH3)3) are used industrially to produce gallium arsenide (GaAs) via the following overall process:

$$AsH3 + Ga(CH3)3 \rightarrow GaAs + 3CH4$$

GaAs is a key component in a wide range of semiconductor-based devices. As in all aspects of the semiconductor manufacturing industry, purity of the chemicals involved at all stages of manufacturing GaAs is a critically important concern. Trace impurities in the process above can substantially affect end use devices.

The focus of this project is to understand the fundamental chemistry associated with the key impurities that are present in the industrial production of arsine using computational quantum chemistry tools. It is surmised that GeH4, H2S, H2O and SiH4 are the precursors for the above mentioned impurities. APCI has established arsine product specifications for these four compounds. It is, however, not completely clear as to what is the basis for these specifications. It is likely that if the relevant process chemistry was better understood, it may be possible to relax some of these specifications, resulting in cost savings in the arsine production process. More importantly, once purity specifications can be made based on rigorous thermochemical data, it will be relatively straightforward to determine if new specifications are needed when end-users alter the conditions under which they use arsine. One current trend in GaAs manufacture is to increase the temperature at which the reaction above is performed. The impact of this change on the role of impurities is currently unknown.