STRUCTURE DETERMINATION OF SILICON CLUSTERS IN THE GAS PHASE: A VIBRATIONAL SPECTROSCOPY AND DFT INVESTIGATION

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Metal clusters are often considered convenient models for studying the interactions occurring at active sites in heterogeneous catalysts and semiconductor clusters have implications to the electronics industry. The properties of small clusters often differ from those of bulk material and cluster characteristics can vary drastically with particle size. Hence, it is essential to have systematic studies over a wide range of cluster sizes.

We employ infrared multiple photon dissociation (IR-MPD) spectroscopy to obtain vibrational spectra of clusters tagged with a noble gas atom in the gas phase. This spectroscopic technique makes use of the Free Electron Laser for Infrared eXperiments (FELIX) and has been shown to be an effective method to probe the structure of transition metal clusters.[a] Comparing the observed infrared spectra to those theoretically predicted for multiple isomers of a single cluster enables accurate structural assignments. Recent results on the structures of silicon clusters will be presented and the effect of doping silicon clusters with transition metal atoms[b] will be discussed.

[a] Fielicke, A.; Kirilyuk, A.; Ratsch, C.; Behler, J.; Scheffler, M.; von Helden, G.; Meijer, G. *Phys. Rev. Lett.* **2004**, *93*, 023401.

[b] Gruene, P.; Fielicke, A.; Meijer, G.; Janssens, E.; Ngan, V. T.; Nguyen, M. T.; Lievens, P. *Chem. Phys. Chem.* **2008**, in press.