Overcoming Uncertainties in Molecular Visualization

Uncertainties are difficult if not impossible to avoid. Capturing data from the analog world almost always results in some form of uncertainty. The amount of uncertainty depends on the method of measurement and its accuracy. When visualizing data that has some associated uncertainty, it is essential to properly process and convey such uncertainty and especially the amount of uncertainty keeping in mind that additional processing steps can amplify the uncertainty. There are various sources of uncertainty, such as numerical limitations or limitations of the capture device. However, there are other sources of uncertainty. Some of these uncertainties stem from model assumptions or limitations of how we translate natural specimens to 3D representations. Molecular structures are one example of this. This talk will illustrate this further and point to some of the solutions.