A detailed and yet compact representation of molecular structures and the inclusion of their properties in formulas and graphs has always been at the heart of chemistry and its innovation paved new routes to chemical research. It can been said that chemistry was the first modern science to create new objects to be studied and, as consequence, needed a new language in addition to word and mathematical formulas. It can be said that Molecular Graphics conventions used routinely nowadays are just another type of chemical language.

The massive increase growth of computer graphics technologies for immersive three dimensional Virtual Reality (IVR) and Human Computer Interaction (HCI) make it a possible nowadays to achieve a further evolution in Molecular Graphics. Indeed, it is now possible to create virtual environments that extend a users' perception and increase his ability to quickly tackle with massive amounts of data from multiple sources and interacting with it. One of the main possibilities created by the application IVR technologies to chemical data is the ability to close the gap between human perception and molecular world coupling visual information with proprioception.

Several well-known molecular graphics editors (e.g. VMD) have been provided recently with experimental plug-ins for use with immersive or interactive technologies. However, partly due to limits in the standardization of the underlying hardware and included APIs and partly to the infancy of dedicated software for “serious” data fruition using VR, a reduced number of standards and dominant paradigms have yet to emerge in the exploitation of such technologies. Another technological conundrum lies in the environments in which to develop such software i.e. if it is better trying to deliver a multiplatform unified environment or instead develop plug-ins on a case by case basis; this has deep implication since it is likely to affect the emergence of new representation paradigms that will complete or replace the existing graphical ones.

In this talk I will show the current effort of our group to deliver a multiplatform IVR molecular viewer (called Caffeine, recently presented on the International Journal of Quantum Chemistry) designed from scratch to exploit new technologies. I will take this opportunity to review the role of visualization and graphics in the chemical sciences and finally I will try to address two questions: (i) there is a major cognitive gain in using IVR in
scientific visualization (in particular for chemistry) and if yes (ii) do we need to think new of new ways of representing data specifically for IVR for any discipline (chemistry in this case)?

**About the Speaker**

Dr Giordano Mancini graduated cum laude in Physical Chemistry in University of Rome “La Sapienza” in 2004. He then started a Ph. D. in Physical Chemistry while working also in the Supercomputing consortium CASPUR in Rome and successfully defended his dissertation in 2007. In 2013 he became fixed term researcher in Scuola Normale Superiore. His research interests include the application of molecular modeling to study the effect of point mutations on proteins, the derivation of classical force fields for different classes of molecular systems and development of algorithms and software for molecular dynamics simulations.

Dr Mancini became interested in Scientific Visualization and application for Virtual Reality for Molecular Sciences upon being awarded a national research grant (FIRB) in the framework of a wider consortium, in 2013. Since then, he has worked to the development of molecular viewer called Caffeine, specifically dedicated to Immersive Virtual Reality technologies.

**Admission is free. All are welcome to attend.**