FROM NUMERICAL WAVEFUNCTIONS TO MOLECULAR GRAPHICS

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The interpretation and mapping of thoughts through numbers is a multi-threaded and demanding problem oriented task. The physical mapping between a real life response and an idea is given by the response function. We make to ourselves pictures of facts.

This presentation will deal with a problem-solving environment in computational chemistry or a toolbox with rapid prototyping elements to assist in the process of portraying chemistry in words and pictures. The gOpenMol toolbox is a multi-platform development environment implemented using both low-level C-language coding and a flexible, extendable and portable Tcl/Tk scripting language. The Tcl/Tk scripting engine enables a full and flexible control of the graphical user interface and a powerful but still easy to use computational engine to access and manipulate the data involved. Using the toolbox it is possible to develop a language to portray reality.