Virtual instruments for molecular sciences: are accuracy and interpretation like the devil and the holy grail?

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Is it possible to turn strongly specialized research in the field of computational chemistry into robust and user friendly aids to experiments and industrial applications? What kind of tools should be created to increase the interaction between researchers with different background and push towards new frontiers in computational chemistry? The terrific advancements in quantum mechanical models, the wide availability of computational and analytic tools are paving the route toward the study of problems that were previously difficult or impossible to solve and let imagine even more ambitioustargetsfor fundamentaland applied research. The combination of new compute-and data-centrictechnologies has turned data analysis from an uncommon and retrospective practice into a proactive process of strategic decision and action. This presentation starts from these premises and proposes a perspective for a new cyberinfrastructure aimed to integrate past developments in theory, algorithms and software with new work-flow management tools, data mining and visualization. We make the case for this approach by means of a few examples dealing with unwieldy data types in molecular modeling and results obtained with different unsupervised learning algorithms. Particular attention will be paied to accurate results and their interpretation in terms of stereo-electronic, dynamic, and environmental effects.

The Virtual Multifrequency Spectrometer: status and perspectives of an undergoing project.

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The impressive advances of computer power, effective and user friendly software and graphical interfaces are leading to the development of a new generation of virtual tools able to deal effectively with the complex systems and phenomena of current interest in the study of molecular systems. Going from collections of numbers for oversimplified models toward vis-a-vis comparison between in silico and in vitro outcomes for real systems together with 3D renderings and natural interfaces should finally overcome the residual diffidence of experimentalists for computer simulations. Among those virtual instruments, we will be concerned here with the multifrequency spectrometer (VMS) our group is developing in the last few years [1], which allows vis-a-vis comparison of experimental spectra with their simulated counterparts and interpretation of the results in terms of the interplay among different well defined effects [2,3]. The main building blocks of this tool are, apart from powerful 3D pre- and post-processing tools, first-principle and semiempirical [4] models based on the density functional theory for the proper treatment of stereo-electronic effects, polarizable atomistic [5] and continuum [6] models to deal with environmental effects, perturbative treatments for describing vibrational averaging effects nuclear motions beyond the harmonic level [7], and stochastic approaches to deal with long-

time contributions [8]. In this presentation I will sketch the present status of the multifrequency spectrometer and the ongoing efforts toward increasing its range of application with special reference to EPR spectroscopy taking nitroxide radical sas model systems. Most of the results were obtained in the framework of the DREAMS project financed by and ERC advanced grant.

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