AVVISO DI CONFERENZA

Il giorno **GIOVEDI' 16 GENNAIO 2020** alle ore **16:00**, nell'aula **1A** dell'edificio **H3** dell'Università di Trieste

il Prof. Vincenzo Barone

della **Scuola Normale Superiore** di Pisa

terrà una conferenza dal titolo:

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

Tutti gli interessati sono cordialmente invitati

Il Direttore del Dipartimento di Scienze Chimiche e Farmaceutiche

Prof. Mauro Stener

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

Vincenzo Barone
Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy

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 ambitious targets for fundamental and applied research. The combination of new compute-and data-centric technologies 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 integration of ongoing developments in theory, algorithms and software with contemporary 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 payed to accurate results and their interpretation in terms of stereo-electronic, dynamic, and environmental effects.