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Publication date:
2017

Document Version
Peer reviewed version

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Citation (APA):

Coriani, S. (2017). Developing Theoretical “Beamlines” for Modern Experiments. Abstract from The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists , Munich, Germany.

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Developing Theoretical “Beamlines” for Modern Experiments

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One powerful way to investigate the molecular world is to study its response to electromagnetic fields. Massive investments have been made, during the last two decades, in the advancement of experimental installations for the detection of increasingly sophisticated light-matter interaction, as exemplified by last generation synchrotron and (x-ray) free electron laser facilities. New ways of probing molecules and materials are emerging, addressing a broad range of scientific problems of both fundamental and applied character. These developments are accompanied by an increasing demand for reliable theoretical and computational methodologies, as an essential component to be able to interpret the experimental results and to retrieve precise quantitative chemical information. An overview of our work on the development of such methodologies will be presented, with particular focus on coupled-cluster based methods for core (x-ray) spectroscopy of both ground and excited states [1-8], photoionization processes and photoelectron spectroscopy [9-10], and both coupled cluster and density functional theory protocols for magnetically induced/chiral effects [11-13].

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