Fonctionnelles de la densité: des systèmes atomiques aux systèmes nucléaires

Rapport sur les contributions

https://indico.in2p3.fr/e/19013

ID de Contribution: **5** Type: **Non spécifié**

Welcome and coffee

lundi 3 juin 2019 10:30 (30 minutes)

Classification de Session: Morning 03/06

ID de Contribution: **6** Type: **Non spécifié**

Introduction

lundi 3 juin 2019 11:00 (15 minutes)

Mme Anne Ealet, director of IPNL
M. Philippe Dugourd, director of ILM
M. Jérôme Margueron, GdR RESANET
M. Karim Bennaceur, for the organizing committee

Classification de Session: Morning 03/06

ID de Contribution: **7** Type: **Non spécifié**

Energy density functional methods for low-energy nuclear structure and reactions (tentative title)

lundi 3 juin 2019 11:15 (50 minutes)

Orateur: BENDER, Michael (IPN Lyon)

Classification de Session: Morning 03/06

ID de Contribution: **8** Type: **Non spécifié**

An introduction to density functional theory

lundi 3 juin 2019 14:00 (50 minutes)

This will be an introduction to density-functional theory, starting from the founding Hohenberg-Kohn and Kohn-Sham theorems to more advanced problems. In particular, we will discuss the history of the development of exchange-correlation functionals, and the availability of such functionals for the study of different physical systems.

Orateur: MARQUES, Miguel (Martin-Luther University of Halle-Wittenberg)

Classification de Session: Afternoon 03/06

ID de Contribution: **9** Type: **Non spécifié**

Ensemble density-functional theory for excited states

lundi 3 juin 2019 14:50 (50 minutes)

I will discuss the basics and recent developments in the field of (time-independent) ensemble density-functional theory for neutral and charged electronic excited states.

Orateur: M. FROMAGER, Emmanuel (University of Strasbourg)

Classification de Session: Afternoon 03/06

ID de Contribution: **10** Type: **Non spécifié**

Coffee

lundi 3 juin 2019 15:40 (30 minutes)

Classification de Session: Afternoon 03/06

ID de Contribution: **11** Type: **Non spécifié**

Dynamics of electrons and nuclei in molecules: Beyond the Born-Oppenheimer approximation

lundi 3 juin 2019 16:10 (50 minutes)

Excited-state dynamics is at the heart of Photophysics and Photochemistry. Nonadiabatic transitions are induced by the strong coupling between electronic dynamics and the ultrafast motion of the nuclei, and are observed in phenomena such as photosynthesis, photovoltaics, and exciton transport in π-conjugated complexes. An essential part of the research efforts in these fields is directed towards developing theoretical and computational approaches to describe conformational changes, energy dissipation, or quantum decoherence, i.e., the signature aspects of excited-state processes. In this context, among the most successful frameworks for molecular dynamics simulations of excited-state processes stand trajectory-based quantum-classical methods, as they give access to the study of complex molecular systems. Trajectory-based approaches combine a classical description of nuclear dynamics with a quantum-mechanical description of electronic dynamics. However, the approximations underlying quantum-classical methods are sometimes severe, and are at the origin of controversies as well as of continuous developments.
In this talk I will present a recently-developed trajectory-based approach to nonadiabatic dynamics [1,2]. The actual numerical scheme has been derived from the exact factorization of the electron-nuclear wavefunction [3], a new framework proposed to investigate, interpret and approximate the coupled dynamics of electrons and nuclei beyond the Born-Oppenheimer approximation. The exact factorization provides a new perspective to analyze nonadiabatic processes: (i) it proposes an alternative [4] to the standard Born-Oppenheimer framework, that pictures excited-state processes in terms of wavepackets moving on and transferring between static potential energy surfaces; (ii) it suggests new interpretations [5] of molecular geometric-phase effects, related to conical intersections; (iii) it provides guidelines for developing simulation algorithms in different [6] nonadiabatic regimes. These points will be discussed during the talk and illustrated on low-dimensional models and molecular systems.

[1] S. K. Min, F. Agostini, I. Tavernelli, E. K. U. Gross, J. Phys. Chem. Lett. 2017, 8, 3048-3055.
[2] S. K. Min, F. Agostini, E. K. U. Gross, Phys. Rev. Lett. 2015, 115, 073001.
[3] A. Abedi, N. T. Maitra, E. K. U. Gross, Phys. Rev. Lett. 2010, 105, 123002.
[4] A. Abedi, F. Agostini, Y. Suzuki, E. K. U. Gross, Phys. Rev. Lett. 2013, 110, 263001.
[5] B. F. E. Curchod, F. Agostini, J. Phys. Chem. Lett. 2017, 8, 831-837.
[6] A. Scherrer, F. Agostini, D. Sebastiani, E. K. U. Gross, R. Vuilleumier, Phys. Rev. X 2017, 7, 031035.

Orateur: AGOSTINI, Federica (Laboratoire de Chimie Physique, Université Paris-Sud)

Classification de Session: Afternoon 03/06

ID de Contribution: **12** Type: **Non spécifié**

Time-dependent DFT: Foundations, Fruition and Failures

mardi 4 juin 2019 09:00 (50 minutes)

I attempt to review the present state of time-dependent density functional theory (TDDFT) [1,2] applied to electronic systems. After a brief view at the mathematical foundations, I discuss the numerical aspects of the method and provide some illustrative examples of its application. I will also show some of the difficulties that plague TDDFT and how they start to be addressed.

[1] Time-dependent Density-Functional Theory, Carsten A. Ullrich, Oxford University Press,2012.
[2] Time-dependent Density-Functional Theory, MAL Marques and EKU Gross, Annu. Rev. Phys. Chem. 55, 427, (2004)

Orateur: NIEHAUS, Thomas (Institut Lumière Matière, Lyon)

Classification de Session: Morning 04/06

ID de Contribution: **13** Type: **Non spécifié**

What can we learn from ultracold atoms about dilute neutron matter?

mardi 4 juin 2019 09:50 (50 minutes)

Orateur: URBAN, Michael (IPN Orsay)

Classification de Session: Morning 04/06

ID de Contribution: **14** Type: **Non spécifié**

Coffee

mardi 4 juin 2019 10:40 (30 minutes)

Classification de Session: Morning 04/06

ID de Contribution: **15** Type: **Non spécifié**

Applications of EDF for astrophysics

mardi 4 juin 2019 11:10 (50 minutes)

Orateur: GULMINELLI, Francesca (LPC/Ensicaen)

Classification de Session: Morning 04/06

ID de Contribution: **16** Type: **Non spécifié**

TBA

mardi 4 juin 2019 14:30 (50 minutes)

Orateur: SAVIN, Andreas (Laboratoire de Chimie Theorique, CNRS at Sorbonne Universite)

Classification de Session: Afternoon 04/06

ID de Contribution: **17** Type: **Non spécifié**

TBA

mardi 4 juin 2019 15:20 (20 minutes)

Orateur: MALLIK, Swagata Mallik (LPC Caen)

Classification de Session: Afternoon 04/06

ID de Contribution: **18** Type: **Non spécifié**

Coffee

mardi 4 juin 2019 15:40 (30 minutes)

Classification de Session: Afternoon 04/06

ID de Contribution: **19** Type: **Non spécifié**

Breaking and restoring symmetries in ab initio many-body formalisms

mardi 4 juin 2019 16:10 (50 minutes)

Orateur: DUGUET, Thomas (CEA/Saclay/SPhN)

Classification de Session: Afternoon 04/06

ID de Contribution: **20** Type: **Non spécifié**

Modeling reactivity at the solid-liquid interface

mercredi 5 juin 2019 09:00 (50 minutes)

To describe reactions occurring at the solid/water interface is currently one of the major challenges in modeling in Heterogeneous Catalysis. It requires a proper depiction of the water solvent together with an adequate description of the surface state. Several approaches are available nowadays in the literature, from continuum models to a full explicit description of the liquid water [1]. We have recently shown that continuum models are key to a proper description of reactions occurring at the electrochemical interface on the formic acid oxidation into CO2 [2]. They also open the door to a proper inclusion of the effect of co-adsorbed anions in thermal heterogeneous catalysis [3]. In both cases, charges are involved and the electrostatic contribution in the major one. When H-bonding between the liquid water and the reactant or intermediate is crucial, continuum models are not sufficient and an explicit inclusion of water molecule is a necessity. As a first step, microsolvation can be an effective approach that allowed us to interpret solvent effect in the conversion of levulinic acid into ɣ-valerolactone [4]. Moving to a full description of reactivity the water/metal interface is still beyond a full complete DFT approach provided the minimal size of the periodic cell that is necessary and the minimal sampling required. A combined QM/MM approach could be a promising strategy [5], but necessitates a new generation of metal/water force field [6]. Nevertheless, being less demanding, inspecting transformations occurring at oxide/water interface is now reachable, as illustrated by our recent work on the stability of ɣ-alumina in water [7].
References:
[1] M. Saleheen, A. Heyden, ACS Catal. 8, (2018), pp. 2188-2194
[2] S. N. Steinmann, C. Michel, R. Schwiedernoch, J.-S. Filhol, P. Sautet, Chemphyschem, 16 (2015), pp. 2307-2311
[3] P. Wang, S. N. Steinmann, G. Fu, C. Michel, and P. Sautet, ACS Catalysis, 7, (2017), pp. 1955–1959
[4] C. Michel, J. Zaffran, A. M. Ruppert, J. Matras-Michalska, M. Jedrzejczyk, J. Grams, P. Sautet, Chem. Comm. 50 (2014), pp. 12450–12453
[5] S. N. Steinmann, P. Sautet, and C. Michel, Phys Chem Cheml Phys, 18, (2016), pp. 31850–31861
[6] S.N. Steinmann, R. Ferreira De Morais, A. W. Götz, P. Fleurat-Lessard, M. Iannuzzi, P. Sautet, C. Michel, J Comp Theo Chem, submitted, (2018)
[7] R. Réocreux, "Biomass derivatives in heterogeneous catalysis: adsorption, reactivity and support from first principles", PhD thesis, (2017)

Orateur: MICHEL, Carine (Laboratoire de Chimie, Ecole Normale Supérieure de Lyon)

Classification de Session: Morning 05/06

ID de Contribution: **21** Type: **Non spécifié**

Selected interdisciplinary aspects of static and time-dependent nuclear DFT

mercredi 5 juin 2019 09:50 (50 minutes)

Orateur: LACROIX, Denis (Institut de Physique Nucléaire)

Classification de Session: Morning 05/06

ID de Contribution: **22** Type: **Non spécifié**

Coffee

mercredi 5 juin 2019 10:40 (30 minutes)

Classification de Session: Morning 05/06

ID de Contribution: **23** Type: **Non spécifié**

Summary talk: On DFT and EDF in finite fermion systems

mercredi 5 juin 2019 11:10 (1 heure)

Examples in various systems. Statics and dynamics.

Orateur: SURAUD, Eric (Université Paul Sabatier)

Classification de Session: Morning 05/06

ID de Contribution: **24** Type: **Non spécifié**

General predictions for the neutron star crustal moment of inertia

mardi 4 juin 2019 12:00 (20 minutes)

The neutron star crustal EoS and transition point properties are computed within a unified metamodeling approach. A Bayesian approach is employed including two types of filters: bulk nuclear properties are controlled from low density effective field theory (EFT) predictions as well as the present knowledge from nuclear experiments, while the surface energy is adjusted on experimental nuclear masses. Considering these constraints, a quantitative prediction of crustal properties can be reached with controlled confidence intervals and increased precision with respect to previous calculations: $\approx 11\%$ dispersion on the crustal width and $\approx 27\%$ dispersion on the fractional moment of inertia. The crust moment of inertia is also evaluated as a function of the neutron star mass, and predictions for mass and radii are given for different pulsars. The possible crustal origin of Vela pulsar glitches is discussed within the present estimations of crustal entrainment, disfavoring a large entrainment phenomenon if the Vela mass is above $1.4M_{\odot}$. Further refinement of the present predictions requires a better estimation of the high order isovector empirical parameters, e.g. K_{sym} and Q_{sym}, and a better control of the surface properties of extremely neutron rich nuclei.

Orateur: CARREAU, Thomas (LPC Caen)

Classification de Session: Morning 04/06

ID de Contribution: **25** Type: **Non spécifié**

Density functional, from nuclei to neutron stars

lundi 3 juin 2019 17:00 (20 minutes)

I will present a meta-modeling of the equation of state for the description of nuclear matter, and its application to neutron stars, where the density can reach several times the saturation density of atomic nuclei (the average density of nuclei). This equation of state is based on the extrapolation of our knowledge in nuclear physics around saturation density, towards high density, encoded in terms of a Taylor expansion of the potential energy. The unknown high order parameters of this expansion have a strong impact at high density, and can therefore be constrained by observations of neutron stars. I will illustrate the case of thermal emission from neutron stars and their constrain on the empirical parameter K_{sym} and Q_{sat}.

Orateur: BAILLOT D'ETIVAUX, Nicolas (IPN Lyon)

Classification de Session: Afternoon 03/06