DEVELOPMENT AND APPLICATION OF DFT

A meeting in honor of Prof. emeritus Henry Chermette

10th November 2017, Lyon – France

PROGRAM

08h45 **OPENING AND WELCOME** - CARLO ADAMO, Chimie Paristech

SESSION 1 - Chair ILARIA CIOFINI, Chimie Paristech

09h00 Unexpected and expected features of the Lembarki-Chermette approximation for the density functional for the kinetic energy
TOMASZ A. WESOLOWSKI - University of Geneva

09h40 Explicit Control Over Spin-States using LFDFT: Quartet G.S. in Tetragonal d^5 Systems Platine
CLAUDE DAUL - University of Fribourg

10h20 **COFFEE-BREAK**

SESSION 2 - Chair CARLO ADAMO, Chimie Paristech

10h50 Density Functional Approximations: Past, Present, Future
MARCEL SWART - University of Girona

11h30 Understanding DFT based chemical reactivity using densities and density matrices
PATRICK BULTINCK - University of Ghent

12h10 Approaching Reality : Modeling Electronic Devices
TIM CLARK - University of Erlangen-Nurnberg

12h50 **HENRY CHERMETTE** - University of Lyon1

13h05 **LUNCH COCKTAIL**

SESSION 3 - Chair LAURENT JOUBERT, University of Rouen

14h30 Variational Principle for Partitioning Molecules into Atomic Contributions
PAUL W. AYERS - Mac Master University

15h10 All-metal Aromaticity and Conceptual DFT
PRATIM K. CHATTARAJ - Indian Institute of Technology Kharagpur

15h50 From conceptual DFT to Molecular Conductivity
PAUL GEERLINGS - Free University of Brussels

16h30 **CONCLUSION AND CLOSURE** - ILARIA CIOFINI, Chimie ParisTech

16h40 **SWEET COLLATION**

Further information: https://dft-2017.sciencesconf.org