International Workshop on First-Principle Quantum Methods and Applications to Dynamical Processes

日時 ： 10月12日(火) 9:35 – 17:30

場所 ： 東北大学大学院 化学第4講義室 (化学大学院講義棟1階)

9:35-9:40 Opening

Chair: Hirohiko Kono (Tohoku U.)

9:40-10:40 Eberhard K. U. Gross (Free U. Berlin)

"Time-dependent density functional theory: Successes and perspectives"

10:40-11:10 Tomohito Otobe (U. Tsukuba)

"Density functional study on the mechanisms of molecular ionization under intense laser fields"

11:10-11:20 Riadh Sahnoun (Tohoku U.)

"Stability of highly charged fullerene: A DFT study"

Chair: Vijay Kumar (Tohoku U.)

11:30-12:00 Ewa Broclawik (Institute of Catalysis and Surface Chemistry, Poland, Tohoku U.)

"Spectral properties of transition metals in extended systems: tungsta "smart windows" and iron enzymes - TDDFT approach"

12:00-12:30 Nurbosyn U. Zhanpeisov (Tohoku U.)

"Interactions of small molecules with transition metal modified silicalites and vanadia supported on titania catalysts: A theoretical ab initio and DFT studies"

Chair: Koichi Ohno (Tohoku U.)

13:40-14:20 Yoshiyuki Kawazoe (Tohoku U.)

"Ab initio study to predict new materials in nanoscale"

14:20-14:50 Balazs Hajgato (Tohoku U.)

"Novel series of giant polycyclic aromatic hydrocarbons: Unexpected electronic structure"

14:50-15:20 Tsuyoshi Kato (Tohoku U.)

"Molecular orbital theory for electronic dynamics in an intense laser field"

Chair: Yuichi Fujimura (Tohoku U.)

15:50-16:20 Angelica Garcia-Zacarias (Free U. Berlin)

"Molecular electronics: Calculating the I-V characteristics of single molecules with DFT"

16:20-16:50 Yukiyoshi Ohtsuki (Tohoku U.)

"Numerical synthesis of optimal laser pulses for manipulating dissociation wave packets of I2- in water"

16:50-17:20 Fabio Pichierri (Tohoku U.)

"DFT studies of cucurbituril macrocycles"

Closing

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