

1/2 journée Séminaires Chimie Théorique

Salle conférence 3eme Est, Bat. A12
Jeudi 30 Mai 2013 à partir de 14 :00

14h00-14h30

M. Nakano (Osaka University, Japan)

Nonlinear optical properties of asymmetric open-shell singlet molecular systems

14h30-14h45

K. Yoneda (Osaka University, Japan)

Open-shell characters and third-order nonlinear optical properties of graphene nanoflakes

14h45-15h00

K. Fukuda (Osaka University, Japan)

Structural dependences of the open-shell characters and second hyperpolarizabilities of pi-conjugated fused-ring hydrocarbons

15h00-15h30

R. Kishi (Osaka University, Japan)

Theoretical study on the electronic structure and third-order NLO properties of open-shellquinoidal oligothiophenes

15h30-16h00

Coffee break

16h00-16h30

Y. Shigeta (Osaka University, Japan)

Car-Parrinello molecular dynamics studies on reaction mechanisms of surface oxidation and nylon-degrading enzyme

16h30-16h45

S. Ito (Osaka University, Japan)

Diradical character based molecular design for efficient singlet fission

16h45-17h15

S.Ramasesha (Indian Institute of Sciences, Bangalore)

Fused Azulenes - Molecular Multiferroics?

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