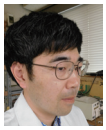
Theoretical Chemistry

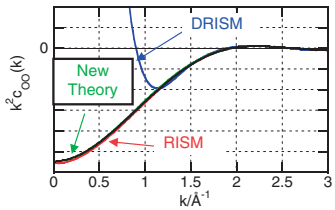
Electrolyte Solutions; DRISM Theory Modifications | Selected Paper | doi:10.1246/bcsj.20150041



T. Yamaguchi

Dielectrically-Consistent Stell Correction for Integral Equation Theory on Electrolyte Solutions

Tsuyoshi Yamaguchi* and Shinobu Koda
Bull. Chem. Soc. Jpn. **2015**, *88*, 804-813

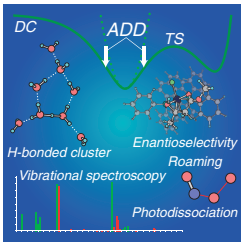


Automated Reaction Path Search Method; GRRM Strategy | OPEN Award Accounts | doi:10.1246/bcsj.20140189

S. Maeda

Anharmonic Downward Distortion Following for Automated Exploration of Quantum Chemical Potential Energy Surfaces

Satoshi Maeda,* Tetsuya Taketsugu, Keiji Morokuma,* and Koichi Ohno*
Bull. Chem. Soc. Jpn. **2014**, *87*, 1315-1334

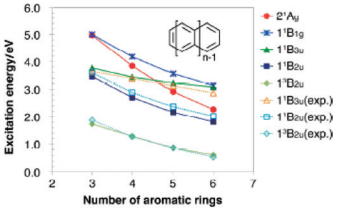


Oligoacenes Excited States; Density Matrix Renormalization Group (DMRG) Method | OPEN BCSJ Award Article | doi:10.1246/bcsj.20140180

Y. Kurashige

Theoretical Study of the π → π* Excited States of Oligoacenes: A Full π-Valence DMRG-CASPT2 Study

Yuki Kurashige* and Takeshi Yanai
Bull. Chem. Soc. Jpn. **2014**, *87*, 1071-1073

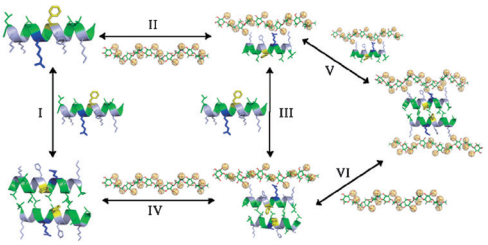


Cell-penetrating Peptides; Heparan Sulfate; MD Simulations | Selected Paper | doi:10.1246/bcsj.20140136

H. Mihara

A Computational Study of the Interaction of Amphiphilic α-Helical Cell-Penetrating Peptides with Heparan Sulfate

Ji Yang, Tadaomi Furuta, Minoru Sakurai, Hiroshi Tsutsumi, and Hisakazu Mihara*
Bull. Chem. Soc. Jpn. **2014**, *87*, 1074-1082

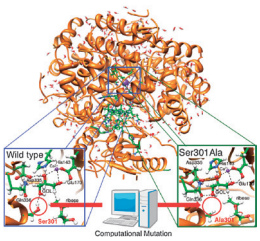


Diol Dehydratase; QM/MM Calculations | Selected Paper | doi:10.1246/bcsj.20140115

K. Yoshizawa

Computational Mutation Design of Diol Dehydratase: Catalytic Ability toward Glycerol beyond the Wild-Type Enzyme

Kazuki Doitomi, Hiromasa Tanaka, Takashi Kamachi, Tetsuo Toraya, and Kazunari Yoshizawa*
Bull. Chem. Soc. Jpn. **2014**, *87*, 950-959

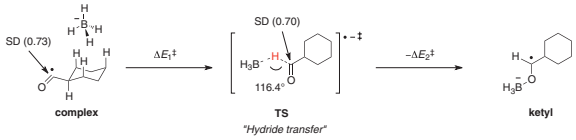


Borohydride Reduction of Acyl Radicals; DFT Calculations | OPEN *Editor's Choice* | doi:10.1246/cl.140370


H. Matsubara

A Theoretical Study on Reduction of Acyl Radicals with Borohydride Anions

Takuji Kawamoto, Hiroshi Matsubara,* and Ilhyong Ryu
Chem. Lett. **2014**, *43*, 1140-1142

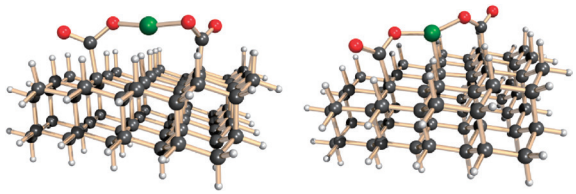


Nanodiamonds Surface; DFT Calculations | *Selected Paper* | doi:10.1246/bcsj.20130345


I. D. Gridnev

Combined Experimental and DFT Study of the Chemical Binding of Copper Ions on the Surface of Nanodiamonds

Ilya D. Gridnev,* Vladimir Yu. Osipov, Alexander E. Aleksenskii, Alexander Ya. Vul', and Toshiaki Enoki
Bull. Chem. Soc. Jpn. **2014**, *87*, 693-704

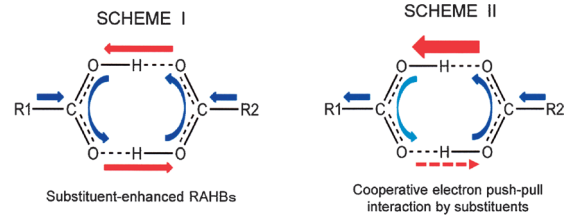


Carboxylic Acid Double H-Bonded Dimers; MP2 Calculations | *Selected Paper* | doi:10.1246/bcsj.20130291


K. Tabayashi

Substituent R-Effects on Intermolecular Resonance-Assisted Hydrogen (H) Bonds: Theoretical Analysis of Double H-Bonded Dimers of Carboxylic Acids

Kiyohiko Tabayashi* and Osamu Takahashi
Bull. Chem. Soc. Jpn. **2014**, *87*, 479-490

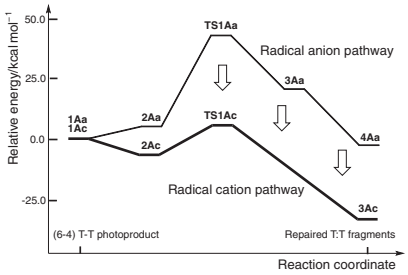


DNA Photoproducts; DFT Calculations | OPEN *BCSJ Award Article* | doi:10.1246/bcsj.20130298


T. Matsubara

Computational Study on the Mechanism of the Electron-Transfer-Induced Repair of the (6–4) T–T Photoproduct of DNA by Photolyase: Possibility of a Radical Cation Pathway

Toshiaki Matsubara,* Nozomi Araida, Daichi Hayashi, and Hatsumi Yamada
Bull. Chem. Soc. Jpn. **2014**, *87*, 390-399

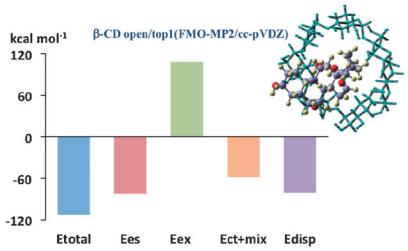


Cyclodextrins Inclusion Complexes; Ab Initio FMO Calculations | *Selected Paper* | doi:10.1246/bcsj.20130205


K. Takano

Theoretical Study on Intermolecular Interactions in Complexes of Cyclodextrins with Bile Acids: DFT and Ab Initio Fragment Molecular Orbital Calculations

Lan Yao, Yukie Mori, and Keiko Takano*
Bull. Chem. Soc. Jpn. **2014**, *87*, 258-266



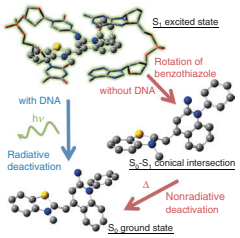
DNA/PicoGreen Complexes; Fluorescence Enhancement Mechanism | Selected Paper | doi:10.1246/bcsj.20130260

H. Nakai

Theoretical Study on the Selective Fluorescence of PicoGreen: Binding Models and Photophysical Properties

Masaki Okoshi, Patchreenart Saparpakorn, Yuta Takada, Supa Hannongbua, and Hiromi Nakai*

Bull. Chem. Soc. Jpn. **2014**, *87*, 267-273



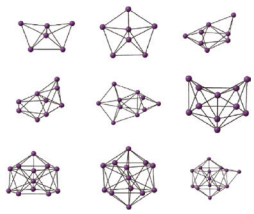
Rb and Cs Atomic Clusters; DFT Calculations | Selected Paper | doi:10.1246/bcsj.20130165

X. Liu

A Density Functional Analysis on Formation of Rubidium and Cesium Atomic Clusters in the Highest Spin State

Xuan Liu,* Haruhiko Ito, and Eiko Torikai

Bull. Chem. Soc. Jpn. **2013**, *86*, 1248-1255



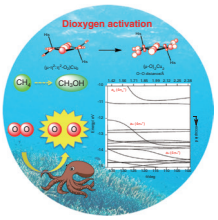
O_2 Activation and CH_4 Hydroxylation by Fe_2, Cu_2 Species; Extended Hückel | OPEN Award Accounts | doi:10.1246/bcsj.20130127

K. Yoshizawa

Quantum Chemical Studies on Dioxygen Activation and Methane Hydroxylation by Diiron and Dicopper Species as well as Related Metal–Oxo Species

Kazunari Yoshizawa

Bull. Chem. Soc. Jpn. **2013**, *86*, 1083-1116



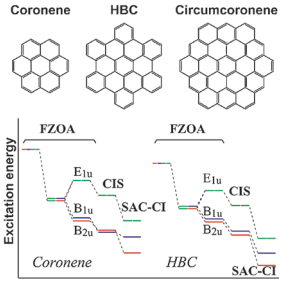
Coronene Excited Electronic States; SAC-CI Method | Selected Paper | doi:10.1246/bcsj.20120317

R. Fukuda

Theoretical Study on the Excited Electronic States of Coronene and Its π-Extended Molecules Using the Symmetry-Adapted Cluster-Configuration Interaction Method

Ryoichi Fukuda* and Masahiro Ehara

Bull. Chem. Soc. Jpn. **2013**, *86*, 445-451



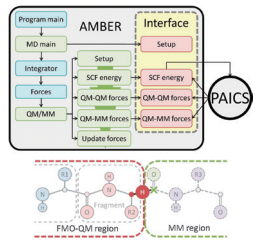
AMBER-PAICS Interface; Ab Initio FMO-QM/MM-MD Simulation | Selected Paper | doi:10.1246/bcsj.20120216

Y. Koyano

A Minimal Implementation of the AMBER-PAICS Interface for Ab Initio FMO-QM/MM-MD Simulation

Takuya Okamoto, Takeshi Ishikawa, Yoshiyuki Koyano, Norifumi Yamamoto, Kazuo Kuwata, and Masataka Nagaoka*

Bull. Chem. Soc. Jpn. **2013**, *86*, 210-222



 doi:10.1246/bcsj.20120243

I. I. Guseinov

Accurate and Fast Evaluation of Three-Center Nuclear Attraction Integrals of Coulomb–Yukawa Like Correlated Interaction Potentials and Slater Type Orbitals

Israfil I. Guseinov and Nurşen Seçkin Görgün*

Bull. Chem. Soc. Jpn. **2013**, *86*, 31-36