

# International Workshop on Molecular Design of Photonic Materials (MDPM99)

## PROGRAM (tentative)

November 11, 1999

### Thursday, December 9

**10:00-10:10**      **Opening Remark**                      Motoi Suwa (ONRI)

**Oral Session 1    NLO: Extended System**

**T-1**    10:10-10:50      *Nonlinear optical responses of strongly correlated system*  
E. Hanamura, N. Trung Dan, and Y. Tanabe

**T-2**    10:50-11:20      *New approaches to modeling the nonlinear optical properties of organic materials*  
D. Yaron, J. Weibel, B. Armitage, and J. Zyss

**T-3**    11:20-11:50      *Theoretical design of molecular aggregates with high static nonlinear optical properties*  
V. M. Yartsev

**T-4**    11:50-12:20      *Nonlinear optical properties of a hypervalent iodine molecule: configuration analysis of hyperpolarizability*  
H. Nobutoki

**12:20-13:20**      **Lunch**

**Oral Session 2    Photo-Induced Process**

**T-5**    13:20-14:00      *An ab-initio MO study on organic photochromic molecules*  
S. Nakamura, D. Guillaumont, F. Pichierri, A. Murakami, K. Kanda, M. Adachi, S. Maeda, K. Mitsuhashi, K. Uchida, and M. Irie

**T-6**    14:00-14:30      *Theoretical study on emission spectra of metal 8-quinolinolato compounds*  
M. Sugimoto, M. Anzai, K. Sakanoue, and S. Sakaki

**T-7**    14:30-15:00      *Theoretical study on the mechanism of electron transfer at photosynthetic reaction centers*  
O. Kitao, K. Aoki, and T. Ogawa

**Oral Session 3    NLO: Vibrational Effect**

**T-8**    15:00-15:30      *Electronic versus vibrational hyperpolarizabilities: structure-property relationships for conjugated organic materials*  
B. Champagne

**T-9**    15:30-16:00      *Intensity-carrying vibrational modes important for nonlinear optical properties derived from algebraic properties of intensity formulas*  
H. Torii

**P-n**    **16:00-18:30**      **Poster Session**

**18:30-20:30**      **Banquet (at room "Oozora-no-ma", 9F)**

### Friday, December 10

**Oral Session 4 NLO: Methodology**

- F- 1** 8:50-9:20 *Time-dependent density functional calculations on frequency-dependent hyperpolarizabilities: current status and future prospects*  
S.J.A. van Gisbergen, E.J. Baerends, and J.G. Snijders
- F- 2** 9:20-9:50 *Dynamic hyperpolarizability calculation without basis functions*  
J. Iwata and K. Yabana
- F- 3** 9:50-10:20 *An efficient quantum chemical program development in material science using quasi particle formalism*  
H. Sekino
- F- 4** 10:20-10:50 *Calculation of dynamic hyperpolarizabilities at the TDHF and MP2 levels based on the quasienergy derivative method*  
T. Kobayashi, M. Shiga, K. Sasagane, F. Aiga, and K. Yamaguchi

**10:50-11:10 Coffee Break**

**Oral Session 5 Excited State Theory**

- F- 5** 11:10-11:50 *Recent advances in electronic structure theory for excited states*  
K. Hirao
- F- 6** 11:50-12:20 *An MO theoretical study of the electronic spectra of  $\pi$ -conjugated systems and the molecular design of functional dyes— the effect of spectrochemical softness on the electronic spectra*  
K. Nishimoto

**12:20-13:20 Lunch**

**Oral Session 6 Two-Photon Absorption**

- F- 7** 13:20-14:00 *Multi-photon absorption and other non linear optical processes studied by analytic response theory calculations*  
H. Ågren, P. Cronstrand, P. Macak, Y. Luo, and P. Norman
- F- 8** 14:00-14:30 *Theory of excitonic two-photon absorption in molecular aggregates*  
S. Abe
- F- 9** 14:30-15:00 *Two-photon absorption in conjugated materials: structure/property relationships*  
D. Beljonne, H. Vögel, T. Kogej, S.R. Marder, J.W. Perry, and J.L. Brédas

**15:00-15:20 Coffee Break**

**Oral Session 7 NLO: Materials Design**

- F-10** 15:20-15:50 *Structure-property correlation of the second hyperpolarizabilities and visualization of its spatial contribution*  
M. Nakano and K. Yamaguchi
- F-11** 15:50-16:20 *Molecular design of donor-acceptor heterocyclic structures for photonics and electronics*  
S. Karna
- F-12** 16:20-16:50 *Design of nonlinear optical materials by molecular orbital methods*

T. Hamada

16:50-17:00

Concluding Remark

Koji Ohta (ONRI)

Closing Remark

Hironobu Okuyama (ONRI)

## POSTER CONTRIBUTIONS

- P- 1** *Adiabatic electronic excitation to a specific vibrational level of diatomic molecule using the delayed pulse method*  
Y. Ohta, T. Yoshimoto, and K. Nishikawa
- P- 2** *Alkyl azide as a source material to photolytically produce a refined beam of neutral radicals*  
M. Fujiyama, A. Maeda, and K. Hayashi
- P- 3** *Computational wavelet model of molecular mechanics for photo sensitive material simulation*  
T. Aratani
- P- 4** *An algebraic probability theory of nonlinear interaction of photon and matter without dipole approximation*  
T. Fukumi
- P- 5** *Calculation of polarizabilities using the full-CI fully variational molecular orbital method*  
M. Tachikawa, K. Sasagane, and Y. Osamura
- P- 6** *PPP molecular orbital calculations of absorption maxima for diarylpolyenes using new- $\gamma$*   
H. Ishihara, F. Noguchi, T. Tachikawa, S. Tokita, I. Iwamoto, K. Hiruta, and K. Nishimoto
- P- 7** *Utilization of the spectrochemical softness parameter evaluated from the absolute hardness to the PPP molecular orbital calculations of the absorption maxima of anthraquinones*  
T. Tachikawa, K. Hiruta, S. Tokita, and K. Nishimoto
- P- 8** *AMI-RPA calculation for predicting UV-visible spectra of some dyes*  
S. Kawauchi, H. Muta, M. Satoh, J. Komiyama, J. Watanabe, Y. Tamura, K. Mori, and K. Suzuki
- P- 9** *MO calculations for absorption spectral changes of dyes from solution to solid state*  
H. Shiozaki, Y. Sakurai, S. Nakao, and M. Kimoto
- P-10** *Excitons and optical absorption spectra in the conjugated polymers PPV and MEH-PPV*  
Y. Matsuzaki, K. Tanaka, T. Yamabe, S. Narita, and T. Shibuya
- P-11** *A first-principles study of polydiacetylene*  
H. Katagiri, Y. Shimoi, and S. Abe
- P-12** *Tetrathiafluvalene derivatives with photochromic diarylethene moieties*  
K. Uchida, G. Masuda, Y. Aoi, and M. Irie
- P-13** *Molecular orbital calculations of substituent effects on conformations of N-benzylideneanilines*  
Y. Kogo, S. Tokita, and K. Nishimoto

- P-14** *Phenylacetylene molecules and dendrimers - ab initio calculations and tight binding model*  
Y. Shimoj and B.A. Friedman
- P-15** *Exciton dynamics in model dendrimers*  
H. Nagao, M. Nakano, K. Kamada, K. Ohta, and K. Yamaguchi
- P-16** *Ab initio calculations of first-order hyperpolarizabilities for donor-acceptor azobenzenes and their dimers*  
Y. Okuno, S. Yokoyama, and S. Mashiko
- P-17** *Ab initio study of substituent effect on SHG-activity of aromatic esters*  
T. Imase, S. Kawauchi, and J. Watanabe
- P-18** *Molecular design of nonlinear optical chromophores for long-term photochemical stability*  
S. Yokoyama, S. Mashiko, Y. Yamaguchi, and Y. Yokomichi
- P-19** *Molecular optical hyperpolarizability of substituted  $\pi$  conjugation system: missing-orbital analysis and simplified sum-over-state calculations*  
M. Tomonari and N. Ookubo
- P-20** *Density functional theory calculations of hyperpolarizabilities of various molecules*  
N. Matsuzawa and D.A. Dixon
- P-21** *Theoretical calculation of hyperpolarizability of molecules with DA-substituents by density functional theory*  
K. Ohta, R. Shikata, K. Kiyohara, K. Tawa, and K. Kamada
- P-22** *Nonlinear optical properties of specific polymethines: influence of substituents and chain length*  
A. Feldner, D. Scherer, M. Welscher, Th. Vogtmann, M. Schwoerer, U. Lawrentz, Th. Laue, H.-H. Johannes, and W. Grahn
- P-23** *Precise comparison of electronic third-order nonlinearity of thiophene homologues by ab initio calculation and femtosecond optical Kerr experiment*  
K. Kamada and K. Ohta
- P-24** *Spatial contribution of virtual excitations to the second hyperpolarizabilities of fractal antenna molecular aggregates*  
H. Fujita, M. Takahata, M. Nakano, S. Kiribayashi, H. Nagao, and K. Yamaguchi
- P-25** *Third-order nonlinear optical properties of fractal antenna molecular aggregates: effects of aggregate architecture*  
M. Takahata, H. Fujita, M. Nakano, S. Kiribayashi, H. Nagao, and K. Yamaguchi
- P-26** *Molecular orbital approach to the surface chemical treatment of CdS ultrafine particles*  
K. Okano, T. Hayashi, and A. Miyamoto
- P-27** *Molecular dynamics simulation study of temperature and density dependence of the optical Kerr effect of liquid carbon disulfide*  
K. Kiyohara, K. Kamada, and K. Ohta
- P-28** *Use of coherent phonon spectroscopy as a probe for distribution of defects in solids*  
K. Ushida, M. Hase, K. Ishioka, and M. Kitajima

- P-29** *Molecular reorientational photorefractive effect in charge-trapping polymer layered liquid crystal*  
J. Mun and C.S. Yoon
- P-30** *Hole transport property of N,N,N',N'-tetraphenyl-(1,1'-biphenyl)-4,4'-diamine and its analogues. A theoretical study*  
K. Sakanoue, M. Sugimoto, M. Motoda, and S. Sakaki
- P-31** *Spectral hole-burning properties of Eu-doped oxide single crystals*  
I. Tanaka, N. Ishii, R. Sato, T. Tamaki, and H. Sasaki
- P-32** *Poly{2,7-bis[2'-(4'-hexylthienyl)]-9,9-dioctylfluorene} — A New Green Fluorescent Polymer for Light-Emitting Diodes*  
B. Liu, W.-L. Yu, Z.-K. Chen, Y.-H. Lai, and W. Huang