# POSTER ABSTRACT REFERENCE

**Poster session (Friday 14:00-16:00)**

**P-1** A numerical approach to obtaining intermediate eigenvalues in electronic structure calculations
*Dongjin Lee, Takafumi Miyata, Tomohiro Sogabe, Takeo Hoshi, and Shao-Liang Zhang*

**P-2** A numerical method for eigenvalue problems in the application of photonic crystals
*Takafumi Miyata, Shao-Liang Zhang*

**P-3** Accelerating electronic structure calculations with mixed precision algorithms
*Eiji Tsuchida and Yoong-Kee Choe*

**P-4** juRS - Massively Parallel DFT in Real-Space
*Paul F. Baumeister, D. Wortmann, S. Bluegel*

**P-5** Development of multisite local orbitals in an O(N) DFT code CONQUEST
*Ayako Nakata, David Bowler, Tsuyoshi Miyazaki*

**P-6** Computational study of the relationship between the molecular and electronic structures of the $Cu_A$ site
*Yu Takano, Orio Okuyama, Yasuteru Shigeta, Haruki Nakamura*

**P-7** Ab initio study of the nucleation of Ge dimers on the {105} facets of a Ge hut
*S. Arapan, D. R. Bowler, and T. Miyazaki*

**P-8** Theoretical study of an natural base pair Ds-Pa in DNA using a linear-scaling DFT method
*T. Otsuka, M. Arita, D. R. Bowler, T. Miyazaki*

**P-9** First-principle calculations of silicene on substrates
*T. Ozaki, C.-C. Lee, H. Kawai, A. Fleurence, R. Friedlein, and Y. Yamada-Takamura*

**P-10** Atomic processes of oxygen plasma etching of graphene surfaces: A Car-Parrinello molecular dynamics study
*Kenichi Koizumi, Mauro Boero, Yasuteru Shigeta, and Atsushi Oshiyama*

**P-11** Floating states that distribute in internal space
*Yu-ichiro Matsushita, Atsushi Oshiyama*

**P-12** Structural exploration by scaled hypersphere search and force inversion
*T. Endo, Y. Gohda and S. Tsuneyuki*

**P-13** A new method to optimize the Jastrow factor using the transcorrelated method and RPA
*Masayuki Ochi and Shinji Tsuneyuki*

**P-14** Ab initio prediction of superconducting transition temperatures based on SCDFT
*Mitsuaki Kawamura, Yoshihiro Gohda, and Shinji Tsuneyuki*

**P-15** Atomistic studies on the reduced thermal conductivity of a thermoelectric clathrate $Ba_8Ga_{16}Sn_{30}$
*T. Tadano, Y. Gohda, S. Tsuneyuki*

**P-16** Effects of imurity hydrogen in rutile $TiO_2$ : Density functional calculation
*Kanako Yoshizawa, Yoshiki Iwazak, Yoshihiro Gohda and Shinji Tsuneyuki*

**P-17** First-principles simulation of water with a hybrid functional computed by graphical processing units
*Yoshihide Yoshimoto*

**P-18** First-principles XPS study on defects: B clusters in Si
*J. Yamauchi, Y. Yoshimoto, and Y. Suwa*

**P-19** Development of first principles molecular dynamics simulation under constant potential bias
*Nicephore Bonnet, Tetsuya Morishita, Osamu Sugino, and M. Otani*

**P-20** Origin of electric double layer at $NaCl_{aq}$ / {Au, Al, MgO} interfaces
*K. Akagi*

**P-21** First-principles study of light emission from silicon and germanium
*Yuji Suwa and Shin-ichi Saito*

**P-22** First principles calculation for electron-phonon dynamics in crystals under ultrashort laser pulses
*Y. Shinohara, S.A. Sato, K. Yabana, T. Otobe, J.-I. Iwata, G.F. Bertsch*

**P-23** Image of helium ion microscopy studied by applying the time-dependent density functional theory
*Yoshiyuki Miyamoto, Hong Zhang, Angel Rubio*

**P-24** Path Integlal simulation for hydrogen bonded systems: Protonic quantum nature and H/D isotiope effect
*Masanori Tachikawa*

**P-25** Quantum Monte Carlo study of the binding of a positron to polar molecules
*Yukiumi Kita and Masanori Tachikawa*

**P-26** The radiative transitions in $TiO_2$-based nanosheets
*Giacomo Giorgi, Maurizia Palummo, Letizia Chiodo, Angel Rubio, Koichi Yamashita*

**P-27** Multiple exciton generation and recombination dynamics in quantum dots
*K. Hyeon-Deuk and O.V. Prezhdo*

**P-28** Symmetric band structures and asymmetric ultrafast electron and hole relaxation dynamics in Si and Ge quantum dots
*K. Hyeon-Deuk and O.V. Prezhdo*

**P-29** Quantum dynamical study of electronic transport through laser-irradiated graphene
*Takashi Akiyama, Matsuto Ogawa and Satofumi Souma*

**P-30** Simulation of AC Response of Defective Metallic Carbon Nanotubes
*Daisuke Hirai, Takahiro Yamamoto, Satoshi Watanabe*

**P-31** Theoretical Study on the Conductive Path in $Cu/Ta_2O_5/Pt$ Atomic Switch
*B. Xiao, T. Tada, T.K. Gu, A. Tawara and S. Watanabe*

**P-32** Electron transport through $\pi$-stack molecular junction
*T. Tada and S. Watanabe*

**P-33** Efficient Relaxation of Magnetic Moments in Noncollinear DFT Calculations
*Marcus Heide, Tomoya Ono*

**P-34** First-principles study on effects of interfacial oxidation in $HfO_2/SiO_2/Si$ interfaces
*Takashi Kojima and Tomoya Ono*

**P-35** Spin dependent transport in boron carbide nitride nanotube
*Huy Duy Nguyen and Tomoya Ono*

**P-36** First-principles study on C removal from 4H-SiC(0001) surfaces and 4H-SiC(0001)/$SiO_2$ interfaces
*S. Saito, S. Sato, Y. Morikawa, and T. Ono*

**P-37** First-principles study and classical molecular dynamics on disorder of 4H-SiC(0001)/$SiO_2$ interfaces
*S.Sato, S.Saito and T.Ono*

**P-38** First principles study of long-range electric transport and thermopower of organometallic complex layers
*H. Nakamura*

**P-39** Bias voltage dependances of STM images of diamino-terphenyl adsorbed on Si(001) surfaces
*Masato Oda*

**P-40** Hydrogen bonding in hydroxyl groups on a metal surface
*Ikutaro Hamada, Takashi Kumagai, Akitoshi Shiotari, Hiroshi Okuyama, Shinichiro Hatta and Tetsuya Aruga*

**P-41** Computational Materials Design from basics to real applications
*H. Kasai, W.A. Dino, H. Nakanishi*

**P-42** Mechanism of hydrazine adsorption and decomposition on metal surfaces
*Mohammad Kemal Agusta, Hideaki Kasai*

**P-43** Structure and stability of borohydride on Au(111) and $Au_3M(111)$ (M = Cr, Mn, Fe, Co, Ni, Cu) surfaces
*Ryan Lacdao Arevalo, Mary Clare Sison Escano, Hideaki Kasai*

**P-44** Effects of Spin-polarization of Pt on Oxygen Dissociative Adsorption
*M.C. Escano, T.Q. Nguyen, H. Nakanishi and H.Kasai*

**P-45** Electronic and Magnetic properties in $Co_{[1ML]}/Ni_{[2ML]}$ multi-layer on W(110)
*K. Kojima, W. A. Dino, M. Suzuki, T. Yasue, K. Kudo, N. Akutsu, E. Bauer, T. Koshikawa and H. Kasai*

**P-46** Molecular Electronic and Vibrational Dynamics Induced by Surface Plasmon
*Kuniyuki Miwa, Mamoru Sakaue, Hideaki Kasai*

**P-47** First principles investigation of work function variation in Cs-W(110) system at different Cs coverage
*A.A.B. Padama, K. Shimizu, Y. Kunisada, H. Nakanishi and H. Kasai*

**P-48** Molecular Orientation and Surface Site Dependence of Dissociative Adsorption of $O_2$/Al(111)
*K. Shimizu, W.A. Dino, H. Kasai*

**P-49** Effects of $H_2$ Hindered Rotational States on the Ortho-Para $H_2$ Conversion on Ag(111)
*Y. Kunisada, H. Nakanishi, W. A. Dino and H. Kasai*

**P-50** Analysis of the structural and electronic properties of $Pr_2NiO_4$ oxide through first principles calculations
*S. M. Aspera, M. Sakaue, T. D. K. Wungu, M. Alaydrus, T. P. T. Linh, H. Kasai, M. Nakanishi and T. Ishihara*

**P-51** The substitution influence on the ferroelectrics about $Pb(Zr,Ti)O_3$
*Kohei Oka, Hiroshi Nakanishi and Hideaki Kasai*

**P-52** First Principles Calculations on the Water and Anion Formation Reactions on Co-Ppy Cluster
*A.G. Saputro, and H. Kasai*

**P-53** Multidimensional Generalized-ensemble Algorithms for Protein simulations
*Ayori Mitsutake*

**P-54** Computational Analysis of Electron Transfer Reaction by Photolyase/Cryptochrome Blue-Light Photoreceptors
*Ryuma Sato and Takahisa Yamato*

**P-55** Robustness Criteria of Hybridization of double-stranded DNA Sequences
*Yusuke Hosaka, Hirotaka Ono*

**P-56** Extended DFT models of the I-DmoI active site reveal the presence of a third metallic binding site
*A.S. Torralba, F.L. Gervasio*

**P-57** Molecular dynamics study of genus and genus distribution in unfolding process of macromolecules
*M. Yamanaka*

**P-58** On-the-fly free-energy reconstruction using logarithmic mean-force dynamics
*T. Morishita, S. G. Itoh, H. Okumura, and M. Mikami*

**P-59** Ab initio derivation of low-energy effective model based on constrained many-body perturbation theory
*Kazuma Nakamura, Yoshihide Yoshimoto, and Shiro Sakai*

**P-60** Derivation of Static Low-energy Effective Models by ab initio Downfolding Method without Double Counting of Coulomb Correlations
*M. Hirayama, T. Miyake and M. Imada*

**P-61** First-principles calculation of magnetocrystalline anisotropy in FePt and MnAl using maximally localized Wannier functions
*Taichi Kosugi*

**P-62** First-principles study on noncollinear magnetism and effects of spin-orbit coupling in 5d pyrochlore oxide $Cd_2Os_2O_7$
*Hiroshi Shinaoka, Takashi Miyake, Shoji Ishibashi*

**P-63** First-principles electronic structures of iron-based superconductors $Ca_4Al_2O_6Fe_2P_2$ and $Ca_4Al_2O_6Fe_2As_2$
*T. Kosugi, T. Miyake and S. Ishibashi*

**P-64** Canted antiferromagnetism in electron-doped $CaMnO_3$ under epitaxial strains
*Hiromasa Ohnishi, Shoji Ishibashi, and Kiyoyuki Terakura*

**P-65** Quasitparitcle self-consistent GW method in the linearized (APW+MTO) method
*Takao Kotani and Hiori Kino*

**P-66** Frustrated electrons on the triangular lattice in a quasitwo- dimentional Mott insulator, $Pd(dmit)_2$ salts
*T. Tsumuraya, H. Seo, M. Tsuchiizu, T. Miyazaki and R. Kato*

**P-67** Time-dependent density-functional simulation of biphenyl molecule under strong laser pulses
*J. Haruyama, C. Hu, and K. Watanabe*

**P-68** First-Principles Study of Dielectric Function of Boron Nitride Nanostructures
*Hiroshi Goto, Jun Haruyama,Chunping Hu.and Kazuyuki Watanabe*

**P-69** Mechnism behind the high thermoelectric power factor of $SrTiO_3$
*K. Shirai and K. Yamanaka*

**P-70** Stable arrangement of impurities of copper in silicon by ab-initio cluclation
*T. Fujimura, K.Shirai*

**P-71** First-principles study of $\alpha$-tetragonal boron
*Naoki Uemura, Koun Shirai*

**P-72** Chalcopyrite semiconductors $CuInS_2$ and $CuAlSe_2$ based ferromagnetic half metals
*M. Shahjahan, T. Oguchi and K. Shirai*

**P-73** Spin-orbit interaction of multi-layer Bi (001) films
*H. Kotaka, F. Ishii and M. Saito*

**P-74** First-principles calculations of hydrogen and lithium impurities in carbon nanomaterials
*Mohammad Shafiul Alam and Mineo Saito*

**P-75** Computational design of photovoltaic materials with self-organized nano-structures
*Y. Tani, K. Sato and H. Katayama-Yoshida*

**P-76** Control of phase separation and magnetism in LiZnAs-based magnetic semiconductors
*K. Sato, D. V. Nguyen and H. Katayama-Yoshida*

**P-77** The interstitial codoping method for dilute magnetic semiconductors
*H. Fujii, K. Sato, and H. K. Yoshida*

**P-78** Computational Materials Design for Superconductivity of Hole-doped Delafossite $CuAlO_2$, $AgAlO_2$ and $AuAlO_2$
*Akitaka Nakanishi and Hiroshi Katayama-Yoshida*

**P-79** Ab initio study on phase transition of carrier-doped BN between zinc-blende and rhombohedral structures
*S. Nishida, H. Funashima, A. Nakanishi, K. Sato and H. Katayama-Yoshida*

**P-80** Study of thermoelectric properties of LaOMCh using abinito calcualtion
*Hiroki Funashima*

**P-81** Design of magnetic anisotropy and its electric field induced variation in the ferromagnetic ultra-thin films
*Y. Taguchi, H. Kato, M. Nakamura, M. Obata, S. Haraguchi, M. Tsujikawa and T. Oda*

**P-82** Electronic Structures of adsorption Tl on the clean Tl/Si(111) surface
*H. Kato, M. Obata, M. Nakamura and T. Oda*

**P-83** Non-equilibrium Green's function method in the Korringa-Kohn-Rostoker method
*M. Ogura and H. Akai*

**P-84** Development of first-principles electronic structure calculation code for large super cell systems by using screened KKR method
*S. Doi, H. Akai*

**P-85** Reformulated optimized effective potentials and its application with static random–phase -approximation correlation
*Taro Fukazawa*

**P-86** A New Extension of Finite Element Method for Electromagnetic Fields in Excitonic Media
*M. Uemoto and H. Ajiki*

**P-87** Enhanced magneto-optical effect in GaGdN/AlGaN magnetic semiconductor double quantum well superlattices
*Yi-Kai Zhou, Shuichi Emura, Shigehiko Hasegawa and Hajime Asahi*