Wednesday Afternoon
Jacek Waluk, Presiding

1:30 (352). Intramolecular excited state proton transfer: The key to photon induced dynamics in protonated aminoacids. Christophe Jouvet, Claude Dedonder, Geraldine Feraud, Gilles Gregoire, Michel Broquier, Satchin Soorkia
2:05 (353) Hydrogen-bond assisted non-radiative decay in solutions and liquid/liquid interfaces. Bogdan Dereka, Sabine Richert, Sandra Mosquera-Vazquez, Eric Vauthey
2:30 (354). Novel, emission-tunable, and ESIPT-capable organic fluorophores. Daniel T Gryko, Lucia Flamigni, Adina Ciuciu, Kamil Skonieczny, Anton J Stasyuk, Michał Cyrański, Barbara Ventura, Marzena Banasiewicz, Bolesław Kozankiewicz
3:05 (355). Investigating ultrafast radiationless decay of a photoacid: Simulating 3-cyano-6-hydroxycoumarin with implicit and explicit ab initio solvent models. SungMin Hong, Ben Nebgen, Lyudmila V. Slipchenko
3:30 INTERMISSION
3:45 (356). Proton shuttle kinetics in a GFP variant switched by pKs changes in a low barrier hydrogen bond. Jie Pan, Mikas Vengris, Deborah Stoner-Ma, Dorte Madsen, Peter J. Tonge, Delmar Larsen
4:20 (357). Designing ESIPT molecules for full-colormolecular pixel system. Soo Young Park, Ji Eon Kwon
4:55 (358). Time-resolved fluorescence study of excited-state proton transfer. Than Htun
5:20 (359). Atypical modulations in the excited state intramolecular proton transfer by diffusive solvent relaxation in room temperature protic ionic liquids. Haridas Pal

Thursday Morning
Bern Kohler, Presiding

8:00 (643). Tautomerism in porphycenes. Jacek Waluk
8:35 (644). Ultrafast IR spectroscopy of photoacid-base complexes: The hydrogen stretching mode as local probe of the hydrogen bond. Brian T Psciuk, Mirabelle Prémont-Schwarz, Benjamin Koeppe, Sharon Keinan, Dequan Xiao, Victor S. Batista, Erik T.J. Nibbering
9:05 (645). Kinetics of excited-state OH^- release from model photobases. Ksenija D Glusac, Yun Xie
9:40 INTERMISSION
9:55 (646). Ultrafast photoionization-induced proton transfer in phenol-ammonia complex. Jr-Wei Ho, Yi-Wei Chen, Ching-Chi Shen, Po-Yuan Cheng
10:30 (647). Detection of ultrafast H atom transfer in the electronic deactivation of the G–C Watson–Crick base pair by femtosecond transient absorption spectroscopy. Katharina Röttger, Friedrich Temps
10:55 (648). Photo-induced redox processes in fluorescent proteins from the GFP family. Anna Krylov
11:25 (649). Firefly bioluminescence: A spectroscopic perspective. Pance Naumov, Kyril M. Solntsev, Sergey Laptenok, Mateusz Rebarz, Oleg V. Maltsev, Lukas Hintermann

Thursday Afternoon
Ksenija Glusac, Presiding

1:30. Photoinduced proton transfer in pyridine based gels: theory and application. Evgenia Vaganova, Ellen Wachtel, David Danovich, Shlomo Yitzchaik, Hans- Helmut Limbach
2:05 (667) Intermolecular charge transfer: A motif for excited-state proton transfer (ESPT). Laren M. Tolbert
2:30 (668). Excited state proton transfer and two color fluorescence of therapeutically potent plant flavonols: Applications toward understanding their interactions with representative bio-relevant targets and nano-vehicles for drug delivery. Pradeep K Sengupta
3:05 (669). Oxyluciferin strong photoacidity in firefly bioluminescence. Luís Pinto da Silva, Joaquim C.G. Esteves da Silva
3:30 INTERMISSION
3:45 (670). Role of photoacid location on proton transfer in confined environments. Nancy E Levinger, Richard L Cole, Myles Sedgwick, Christopher D Rithner, Debbie C Crans
4:20 (671). Mid-IR absorption spectroscopy of hydrogen-bonded complexes in ground and excited electronic states of photoacids Dina Pines, Philip M. Kiefer, James T. Hynes, Ehud Pines
4:55 (673). Elucidation of the dynamic role of alcohol molecular clusters in non-aqueous acid-base reactions. Oh-Hoon Kwon

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August 10-14, 2014

Sunday Morning
Luis Pérez Lustres, Presiding

8:00. Introductory Remarks
8:10 (15). Red-shifted fluorescent proteins with a large Stokes shift: Chemical mechanism and imaging applications of LSSmOrange. Daria M Shcherbakova, Sergei Pletnev, Kiryl D Piatkevich, Vladislav V Verkhusha
8:35 (16). Modeling excited-state intramolecular proton transfer with TD-DFT. Adèle D Laurent, Ymène Houari, Denis Jacquemin
9:05. Charge-bond resonance in fluorescent protein chromophore motifs: Implications for excited-state proton transfer and its coupling to photoisomerization behaviour. Seth Olsen
9:40 INTERMISSION
9:55 (18). Proton-coupled electron/hole transfer in DNA damage induced by one-electron oxidation of guanine. Vladimir Shafirovich, Nicholas E Geacintov
10:25 (19). Mid-infrared spectroscopy for ground and excited state proton transfer in phenol/naphthol-ammonia clusters. Masaaki Fujii
10:50 (20). Ultrafast dynamics of proton transfer and twisting motion in a salicylideneaniline derivative in solution and within NaX and NaY zeolites. Noemi Alarcos, Boyko Cohen, Juan Angel Organero, Felix Sanchez, Abderrazzak Douhal
11:25 (21). Juggling with protons: From theory to applications. Andrzej L. Sobolewski

Sunday Afternoon
Omar Mohammed, Presiding

1:30 (69). Proton-coupled electron transfers: pH-dependent driving forces? Fundamentals and artifacts. Marc Robert
2:05 (70). Surface hopping dynamics of excited-state proton transfer. Walter Thiel
2:30 (71). Exploring the photochromism of new salicylideneanilines in different environment with transient spectroscopies and chemometric modeling. Michel Sliwa, Bruno Debus, Gotard Burdzinski, Pance Naumov, Pei Yu, Cyril Ruckebusch
3:05 (72). Watching protons move by ultrafast continuum mid-IR spectroscopy. Ashley M Stingel, Brian V Hoozen, Poul B Petersen
3:30 INTERMISSION
3:45 (73). Development of ESIPT-based fluorescent L-amino acid analogs: Applications in monitoring protein/ligand interactions Yves Mely, Viktoriia Y Postupalenko, Volodymyr V Shvadchak, Marianna Sholokh, Andrey S Klymchenko, Aleksandr V Strizhak, Oleksandr M Zamotaiev, Vasyl G Pivovarenko
4:20 (74). Long-lived reversible photoacids: Application to energy propagation throughout a chemical network. Matthieu Emond, Ahmed Alouane, Frédéric Schmidt, Thomas Le Saux, Raphaël Plasson,Ludovic Jullien
4:55 (75). Nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes. Sharon Hammes-Schiffer
5:20 (76). Proton-transfer via protein-bound water molecules in biomembrane transporters. Steffen Wolf, Klaus Gerwert

Monday Morning
Adele Laurent, Presiding

8:00 (125). Excited-state proton transfer in a calcium-sensing fluorescent protein complex: Structural dynamics insights from femtosecond stimulated Raman spectroscopy. Breland G. Oscar, Weimin Liu, Yongxin Zhao, Longteng Tang, Yanli Wang, Robert E. Campbell, Chong Fang
8:35 (126). Excited state proton transfer reactions and DFT: Old and new challenges. Nadia Rega, Ilaria Ciofini, Carlo Adamo, Alessio Petrone, Marika Savarese, Greta Donati, Umberto Raucci
9:05 (127). Photoacids under investigation: Theoretical modeling of excited state proton transfer to solvent in solvent. Lyudmila V. Slipchenko, SungMin Hong, Ben Nebgen
9:40 INTERMISSION
9:55 (128). Adapted spherically-symmetrical Brownian dynamic models as a tool for simulations of the reversible proton transfer in highly asymmetric systems. Alexander V. Popov, Kyril M. Solntsev, Rigoberto Hernandez
10:30 (129). Electron and proton transfer from tyrosine and tryptophan residues in azurin. Judy E. Kim, Bethany C. Larson, Jennifer R. Pomponio, Hannah S. Shafaat, Rachel H. Kim, Brian S. Leigh, Michael J. Tauber
10:55 (130). Smart hydogel using pH-jump reaction with PAG for biomedical application. Takao Aoyagi, Misuhiro Ebara
11:30 (131). Elementary steps in proton transfer to solvent. Jorge A Pedro, Flor Rodríguez-Prieto, M. Carmen Ríos Rodríguez, Manuel Mosquera, J. Luis Pérez Lustres

Monday Afternoon
Steven Boxer, Presiding

1:30 (183). Hidden photoinduced proton transfer in the Blue Fluorescent Protein mKalama1: Theoretical insight. Anastasia V. Bochenkova, Kyril M. Solntsev
2:05 (184) Excited-state water catalyzed proton transfer reaction: Fundamental and biomedical applications. Pi-Tai Chou
2:30 (185). How fast a proton transfer reaction can be? Beyond the solvent control limit. Dan Huppert, Ron Simkovitch, Shay Shomer, Rinat Gepshtein
3:05 (186). Proton-coupled electron transfer during the S-state transitions of the oxygen-evolving complex of photosystem II. Muhamed Amin, Sergey Vassiliev, Leslie Vogt, Gary Brudvig, Doug Bruice, Marilyn Gunner
3:30 INTERMISSION
3:45 (187). Photo-control of pH-driving processes with reversible metastable-state photoacids. Yi Liao
4:20 (188). Simulations of proton transfer routes in proteins of the green fluorescent protein family. Alexander Nemukhin, Bella Grigorenko, Valdimir Mironov
4:55 (189). "Turn on/off" proton transfer based fluorescent chemosensor for detection of environmentally hazardous metal ions. Papia Chowdhury, Nidhi Singla
5:20 (190). Proton-coupled electron transfer with photoexcited metal complexes. Oliver S. Wenger

Tuesday Morning
Noam Agmon, Presiding

8:00. Thermodynamic correlations between amino-type excited-state intramolecular proton transfer, proton-donor/acceptor capabilities, and hydrogen-bond strengths. Huan-Wei Tseng, Jun-Qi Liu, Yi-An Chen, Chi-Lin Chen, Tian-Lin Wang, Kuan-Miao Liu, Chimin Chau, Pi-Tai Chou
8:35 (239). Excited state intramolecular hydrogen transfer (ESIHT) of 1,8-dihydroxy-9,10-anthraquinone (DHAQ) characterized by ultrafast electronic and vibrational spectroscopy and computational modeling. Omar F. Mohammed, Erik T. J. Nibbering, Dequan Xiao, Victor S. Batista
9:05 (240). GFP does ESPT - split GFPs do many things. Steven Boxer
9:40 INTERMISSION
9:55 (241). Excited-state multiple proton transfer in hydrated 7-azaindole clusters in the gas phase. Kenji Sakota, Gustavo A Pino, Claude Dedonder, Christophe Jouvet, Hiroshi Sekiya
10:30 (242). Photoinduced proton-coupled electron transfer in model DNA helices. Bern Kohler, Yuyuan Zhang, Kimberly de La Harpe
10:55 (243). Mimics of the Tyr_Y-His redox relay of photosystem II. Ana L Moore, Devens Gust, Thomas A. Moore, Manuel J. Llansola-Portolés, Gerdenis Kodis, Dalvin D. Méndez-Hernández, John Tomlin
11:30 (666). Photoinduced fragmentation of protonated peptides: Following the bouncing proton. Nicole L Burke, Jacob C Dean, Scott A McLuckey, Timothy S Zwier

Wednesday Morning
Laren Tolbert, Presiding

8:00 (299). Theory of proton vibrational stretch frequencies in solution phase acid-base hydrogen-bonded complexes in ground and excited electronic states. Philip M. Kiefer, Ehud Pines, Dina Pines, James T. Hynes
8:35: Probing Water Dynamics the Missing Link for Understanding Protein Structure-Catalysis and Signaling Transduction. Hsiao-Ching Yang
9:10 (301). Proton coupled electron transfer reactions in photosynthesis and biomimetics. Bridgette A Barry
9:40 INTERMISSION
9:55 (302). Proton migration and privileged water exchange in the green fluorescent protein. Ai Shinobu, Noam Agmon
10:30 (303). Proton-transfer-induced modification on firefly bioluminescence. Young Min Rhee, Hyun Woo Kim
10:55 (304). Excited state proton transfer in a live lung cell: Normal and cancer cell. Rajdeep Chowdhury, Abhijit Saha, Amit K Mandal, Batakrishna Jana, Surajit Ghosh, Kankan Bhattacharyya
11:30 (305). Correlation between excited-state intramolecular proton-transfer and singlet-oxygen quenching activity in intramolecularly hydrogen-bonded anthraquinone derivatives. Shin-ichi Nagaoka, Hikaru Endo, Keishi Ohara