THURSDAY MORNING * ROOM 29C

Adam Willard, Presiding

8:00 (607). From dimers to self-assembled molecular nanotubes: Challenges for theory. **A. Stradomska**

8:30 (608). Living on the edge: Tuning supramolecular interactions to design two-dimensional organic crystals near the boundary of two stable structural phases. B. Hirsch, K.P. McDonald, B. Qiao, A.H. Flood, **S.L. Tait**

8:50 (609). Self-assembly of hierarchical biomorphs from crystalline nanorods. **E. Nakouzi**, P. Knoll, Y. Ghoussoub, O. Steinbock

9:10 (610). Atomistic simulations of the formation of perylene-based supramolecular complexes in aqueous solution. **N. Hansen**

9:30 INTERMISSION

9:40 (611). Light harvesting in purple bacteria benefits more from a favorable energy landscape than from coherent delocalization. S. Baghbanzadeh, **I. Kassal**

10:10 (612). Withdrawn

10:30 (613). Effective optoelectrical switching by using pseudo-single crystal of monolayer array of 2D polymer-plasmonic nanoparticles system. **M.A. Mahmoud**

10:50 (614). Enol tautomeric polymorph of barbituric acid: The role of zero point energy in stability. **B.S. Hudson**, M. Marshall, V. Lopez, D.G. Allis

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251st National ACS Meeting

Division of Physical Chemistry

Supramolecular Aggregates: Fundamentals & Applications of Soft Self-Assembled Materials

Dorthe M. Eisele

Adam P. Willard

Organizers

March 14-17, 2016

San Diego Convention Center

ROOMS 29D/C/B

MONDAY MORNING * ROOM 29D

Dorthe M. Eisele, Presiding

8:00 (135). Elucidation of the molecular machinery in photosynthetic light harvesting. **G. Schlau-Cohen**
8:30 (136). Many-body dispersion and its effect in the interactions of organic chromophores and two-dimensional materials. **A. Aspuru-Guzik**
9:00 (137). Engineering nanometer-scale coherence in soft matter. **C. Liu**, Y. Zhang, P. Zhang, D.N. Beratan
9:20 INTERMISSION
9:40 (138). Balance of order and disorder as the key to tailor various properties of soft materials. **H. Frauenrath**
10:10 (139). Photophysics of self-assembled carotenoid aggregates. **M.J. Tauber**, S. Doyle, C. Wang

MONDAY AFTERNOON * ROOM 29C

Seogjoo Jang, Presiding

1:30. Dihalopolydiacetylenes: Supramolecular Synthesis, Aggregation, and Properties. **N. S. Goroff**, M. Freitag, H. Jin, U. Salisu, D. Yang, M. Eisaman, and A. Ashraf
2:00 (182). Energy transport in nanotubular supramolecular cyanine aggregate systems. **D.A. Vanden Bout**, E.L. Kreuger
2:20 (183). Mobility of excitons in perylene bisimide aggregates. **F. Fennel**, S. Wolter, S. Lochbrunner, F. Wuerthner
2:40 (184). Infrared invisibility stickers inspired by cephalopods. L. Phan, D.D. Ordinario, E. Karshalev, W. Walkup IV, M. Shenk, **A.A. Gorodetsky**
3:00 INTERMISSION
3:10 (185). Molecular simulations of π-π stacking mediated self-assembly in supramolecular filaments. M. Kang, P. Zhang, H. Cui, **S. Loverde**
3:40 (186). Understanding and designing self-assembled molecular J-aggregates for long-range coherent energy transport. **J. Caram**, D.M. Eisele, S. Doria, S. Lloyd, M.G. Bawendi
4:00 (187). Interchain charge-transfer states facilitate triplet formation in polymer aggregate nanofibers. **A. Thomas**, J. Garcia-Galvez, H.A. Brown, J.K. Grey

TUESDAY MORNING * ROOM 29B

Sharon Loverde, Presiding

8:00 (230). Dynamic peptide libraries for materials discovery. **R. Ulijn**
8:30 (231). Generalized master equation approach for coarse grained exciton dynamics in supramolecular systems. **S. Jang**
9:00 (232). DFT-NEGF study of conducting protein filaments for solar energy harvesting. **H.P. Hendrickson**, N.S. Malvankar, V.S. Batista
9:20 (233). Correlating spectral shifts, polarization, and molecular orientation in conjugated organic thin films and microstructures. **J.M. Szarko**, A. Austin, X. Zhu
9:40 INTERMISSION
9:50 (234). Bio-inspired supramolecular materials. **S.I. Stupp**
10:20 (235). Photophysical and electrochemical properties of perylene bisimide homo- and heterodimers. **A. Nowak-Król**, B. Fimmel, M. Son, D. Kim, F. Wuerthner
10:40 (236). *In situ* liquid cell TEM observations of the size evolution pathways of amphiphilic polymer micelle nanoparticles. **L.R. Parent**, J.K. Kammeyer, J.P. Patterson, E. Bakalis, F. Zerbetto, C. Park, N.C. Gianneschi
11:00 (237). Excitonic structure and environment effects in porphyrin aggregates probed with low-temperature fluorescence. **C.W. Leishman**, J. McHale

WEDNESDAY MORNING * ROOM 29C

Bohdana Discher, Presiding

8:00 (300). Self-assembly and mechanical properties of a physically associating gel. **S. Kundu**, S. Hashemnejad, M. Zabet, S. Mishra
8:30 (301). Controlling interchromophore coupling in symmetric dimers: The role of bridge's electronic structure. **C. Cruz**, P. Christensen, E.L. Chronister, D. Casanova, M.O. Wolf, C.J. Bardeen
8:50 302). Exploring the relationship between cage forming ligands and the network structure of their gels. **E. Alt**, A.P. Willard
9:10 INTERMISSION
9:20 (303). Self-assembled nano-containers assembled via the hydrophobic effect. **B.C. Gibb**
9:50 (304). Revealing relationships between conformation and photophysics in single conjugated polymers and aggregates. **D.T. Hoang**, J. Yang, H. Park, L. Kaufman
10:10 (352). Three dimensional self-assembled monolayers around nanodroplets for lipid studies. Y. Chen, C. Luetgebaucks, H. Okur, **S. Roke**

WEDNESDAY AFTERNOON * ROOM 29C

Rein Ulijn, Presiding

1:30 (351). Photophysical properties of multichromophoric architectures of perylene bisimide dyes. **F. Wuerthner**

2:00 (305) Molecular dynamics study of self-assembly of low molecular mass organic gelators. M. Huda, **N. Rai**

2:20 (358). Designing multiscale models for self-assembling peptide **M. McCullagh**, P. Lake

2:40 (354). Huddling together when something is missing: Supramolecular aggregation in monolacunary Keggin anions. **S. Serapian**, A. Neyman, C. Bo, I.A. Weinstock

3:00 INTERMISSION

3:10 (355). Supramolecular self-assembly of amphiphilic synthetic redox proteins. B.A. Fry, G. Goparaju, C.C. Moser, P. Dutton, **B.M. Discher**

3:40 (356). Phase behavior of complex lipid mixtures: Signatures of spatial organization. S. He, K. Sapp, **L. Maibaum**

4:00 (357). Role of environmental conditions on the photochemica synthesis and self-assembly of amphiphiles in aqueous solution. **R. Rapf**, R. Perkins, V. Vaida

4:20 (353). Discerning the effect of counter ions on supramolecular self-assembly. **S.J. Belh**, K. Ng, G. Huffman, A. Chowdhury, N. Yehya, D.M. Eisele