

ICCC2018 Program (S16)

| July 30, 2018 (Mon) |   | July 31, 2018 (Tue)                        |                | Aug 1, 2018 (Wen)                            |          | Aug 2, 2018 (Thu)                                 |                | Aug 3, 2018 (Fri)                              |       | Aug 4, 2018 (Sat)                                 |  |
|---------------------|---|--|----------------|--|----------|---|----------------|--|-------|---|--|
|                     | 8:30  | Plenary Lecture<br><b>Prof. Yi Lu</b>      | 8:30           | Plenary Lecture<br><b>Prof. Gary Brudvig</b> | 8:30     | Plenary Lecture<br><b>Prof. Roland A. Fischer</b> | 8:30           | Plenary Lecture<br><b>Prof. Shie-Ming Peng</b> | 8:30  | Plenary Lecture<br><b>Prof. Mario Ruben</b>       |  |
|                     | 9:15  | Coffee Break                               | 9:15           | Coffee Break                                 | 9:15     | Coffee Break                                      |                |  |       |   |  |
|                     | 9:40  | Larry Que                                  | 9:40           | Ken Karlin                                   | 9:40     | Shunichi Fukuzumi                                 |                |  |       |   |  |
|                     | 10:05   | Julie Kovacs                               | 10:05          | Masahito Kodera                              | 10:05    | Tai-Chu Lau                                       |                |  |       |   |  |
|                     | 10:25   | Takahiko Kojima                            | 10:25          | Dan Stack                                    | 10:25    | Mike Green  |                |  |       |   |  |
|                     | 10:45   | Toshitaka Matsui                           | 10:45          | Yasuhiro Funahashi                           | 10:45    | Huantian Shi                                      |                |  |       |   |  |
|                     | 11:00   | Jun Nakazawa                               | 11:00          | Tsukasa Abe                                  | 11:00    | Tohru Wada  |                |  |       |   |  |
|                     | 11:15   | Shiro Hikichi                              | 11:15          | Syuhei Yamaguchi                             | 11:15    | Yasuyuki Yamada                                   |                |  |       |   |  |
|                     | 11:30   | <b>Mónica Rodríguez</b>                    | 11:30          | T. Misawa-Suzuki                             | 11:30    | Shinya Ariyasu                                    |                |  |       |   |  |
|                     | 11:45   | Koji Oohora                                | 11:45          | Nanda Dulal Paul                             | 11:45    | Kei Ohkubo  |                |  |       |   |  |
|                     | 12:00   | Santiago Alvarez                           | 12:00          |  | 12:00    |   |                |  |       |   |  |
|                     | 12:15   | Lunch                                      | 12:15          | Lunch  |          |   |                |  | 12:10 | <b>Special Lecture: Prof. Jean-Pierre Sauvage</b> |  |
|                     | 13:15   | Plenary Lecture<br><b>Prof. Lee Cronin</b> | 13:15          | Plenary Lecture<br><b>Prof. Hideo Hosono</b> |          |   | 13:15          | Plenary Lecture<br><b>Prof. James Mayer</b>    |       |   |  |
|                     | 14:00   | Coffee Break                               | 14:00          | Coffee Break                                 |          |   |                |  |       |   |  |
|                     | 14:25   | Wonwoo Nam                                 | 14:25          | Chris Cramer                                 |          |   |                |  |       |   |  |
|                     | 14:50   | David Goldberg                             | 14:50          | Yoshihito Shiota                             |          |   |                |  |       |   |  |
|                     | 15:10   | Hiroshi Fujii                              | 15:10          | Kallol Ray                                   |          |   |                |  |       |   |  |
|                     | 15:30   | Tapan Kanti Paine                          | 15:30          | Christian Linberg                            |          |   |                |  |       |   |  |
|                     | 15:50   | X. Engelmann                               | 15:50          | Hiroaki Kotani                               | 12:15    | Excursion   |                |  |       |   |  |
|                     | 16:05   | G. Olivo                                   | 16:05          | C. Carlota                                   |          |   |                |  |       |   |  |
|                     | 16:20   | Coffee Break                               | 16:20          | Coffee Break                                 |          |   |                |  |       |   |  |
|                     | 16:45   | Andy Borovik                               | 16:45          | Tim Warren                                   |          |   |                |  |       |   |  |
|                     | 17:10   | Way-Zen Lee                                | 17:10          | Todd Harrop                                  |          |   |                |  |       |   |  |
|                     | 17:30   | Shengfa Ye                                 | 17:30          | Guochuan Yin                                 |          |   |                |  |       |   |  |
|                     | 17:50   | <b>N. C. Mösch-Zanetti</b>                 | 17:50          | Y. Arikawa                                   |          |   |                |  |       |   |  |
| 18:00               | <b>Special Lecture: Prof. Akira Fujishima</b> | 18:05                                      | Yuma Morimoto  | 18:05  | T. Toshi |   |                |  |       |   |  |
|                     |   | 18:20                                      | P. Vijayendran | 18:20  |          |   |                |  |       |   |  |
|                     |   | 18:35                                      | End            | 18:35  | End      | 18:30   | Poster Session |  |       |   |  |

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| 18:30 | <b>Poster Session of S16<br/>(this session)</b> |
|       |   |
| 20:30 |   |

| Session | Lecture   | Poster Date | Code      | Name              | Affiliation  | Title  |
|---------|-----------|-------------|-----------|-------------------|--|--|
| S16     | Organizer |             |           | Shinobu Itoh      | Osaka University   |  |
| S16     |           |             |           | Takahiko Kojima   | University of Tsukuba                                    |  |
| S16     |           |             |           | Wonwoo Nam        | Ewha Womans University                                   |  |
| S16     |           |             |           | A. S. Borovik     | University of California-Irvine                          |  |
| S16     |           |             |           | Franc Meyer       | Georg-August-University Göttingen                        |  |
| S16     | Keynote   |             | A00347-CC | Chris Cramer      | University of Minnesota                                  | Activation of C-H Bonds by the Cu(III)OH Functional Unit   |
| S16     | Keynote   |             | A02092-SF | Shunichi Fukuzumi | Ewha Womans University                                   | Production and Utilization of Liquid Solar Fuels   |
| S16     | Keynote   |             | A05038-WN | Wonwoo Nam        | Ewha Womans University                                   | Metal-Oxygen Intermediates in Dioxygen Activation Chemistry  |
| S16     | Keynote   |             | A02193-AB | Andy S. Borovik   | University of California-Irvine                          | Metal-Oxido and Hydroxido Complexes: Intermediates in Water Oxidation and Dioxygen Activation  |
| S16     | Keynote   |             | A02232-KK | Kenneth Karlin    | Johns Hopkins University                                 | Nitrogen Oxide Chemistries with Copper or Heme Complexes: Bioinorganic Aspects   |
| S16     | Keynote   |             | A03033-LQ | Larry Que         | Department of Chemistry, University of Minnesota         | The Amazing High-Valent Iron-Oxo Landscape   |
| S16     | Keynote   |             | A03069-TW | Tim Warren        | Department of Chemistry, Georgetown University           | Nitric Oxide Activation at Mononuclear Cu and Ni Sites   |
| S16     | Invited   |             | A03066-JK | Julie Kovacs      | Department of Chemistry, University of Washington        | The Influence of Thiolate Ligands on Iron Dioxygen Chemistry   |
| S16     | Invited   |             | A03070-MG | Michael Green     | University of California-Irvine                          | Selenocysteine Cytochrome P450 Compound I: A Direct Link Between Electron Donation and Reactivity  |
| S16     | Invited   |             | A02174-DG | David Goldberg    | Johns Hopkins University                                 | Direct Observation of Radical Rebound with an Iron Hydroxide Complex   |
| S16     | Invited   |             | A00910-HF | Hiroshi Fujii     | Nara Women's University                                  | Heterolytic versus Homolytic Bond Cleavage of Hypochlorite by Iron Porphyrin Complexes   |
| S16     | Invited   |             | A03071-TP | Tapan Kanti Paine | Indian Association for the Cultivation of Science (IACS) | Effect of Second Coordination Sphere on the Reactivity of Iron(III)-Alkylperoxide Intermediates: Implications for Selective Catalytic Oxidations |
| S16     | Invited   |             | A03072-WL | Way-Zen Lee       | National Taiwan Normal University                        | Synthesis and Reactivity of Well Characterized Nonheme Manganese(III)-Superoxo Complexes   |
| S16     | Invited   |             | A03073-SY | Shengfa Ye        | Max-Planck Institutur fur Kohlenforschung                | Characterization of Novel Intermediates Derived from Dioxygen Activation   |
| S16     | Invited   |             | A01006-MK | Masahito Kodera   | Doshisha University                                      | Hydroxylation of inert hydrocarbons catalyzed by bioinspired dicopper complexes stabilized by dinucleating ligands                               |
| S16     | Invited   |             | A02135-DS | Dan Stack         | Stanford University                                      | Imidazole Ligation of Cu(I) in the Activation of Dioxygen: The Role of Cu(III)   |
| S16     | Invited   |             | A05036-YS | Yoshihito Shiota  | Kyushu University  | Theoretical Study of Methane Activation at the Dicopper Site of pMMO   |
| S16     | Invited   |             | A02012-KR | Kallol Ray        | Humboldt University Berlin                               | SMALL MOLECULE ACTIVATION AT TRANSITION METAL CENTERS: STRUCTURE-FUNCTION CORRELATIONS   |
| S16     | Invited   |             | A01196-CL | Christian Limberg | Humboldt-Universitat zu Berlin                           | Structural and functional models for the 1-aminocyclopropane-1-carboxylic acid oxidase   |

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| S16 | Invited   |  | A02011-TH | Todd Harrop          | University of Georgia, Department of Chemistry and Center for Metalloenzyme Studies      | Metal Complexes Involved in NO <sub>x</sub> Transformations Related to Global Nitrogen                                      |
| S16 | Invited   |  | A03074-GY | Guochuan Yin         | Huazhong University of Science and Technology  | Oxidative relationships of active metal oxo and hydroxo species and its implications to catalyst design                     |
| S16 | Invited   |  | A00860-TL | Tai-Chu Lau          | City University of Hong Kong   | Reactivity of some d <sup>2</sup> nitrido complexes   |
| S16 | Invited   |  | A01519-TK | Takahiko Kojima      | Department of Chemistry, Faculty of Pure and Applied Sciences, University of Tsukuba     | Catalytic Oxidation by Ruthenium-Oxo and -Oxyl Complexes Using Water as an Oxygen Source                                    |
| S16 | Oral Talk |  | A01393-TM | Toshitaka Matsui     | Tohoku Univ.   | Unique heme degradation mechanism of IsdG from <i>Staphylococcus aureus</i>   |
| S16 | Oral Talk |  | A01720-JN | Jun Nakazawa         | Kanagawa University  | Alkane Oxidation by Homogeneous and Immobilized Ni(II) Complex Catalysts with BOX-type Ligands                              |
| S16 | Oral Talk |  | A01653-SH | Shiro Hikichi        | Kanagawa University  | Non-heme iron complexes with bis(imidazolyl)borate ligands for mimicking biological O <sub>2</sub> -activating iron sites   |
| S16 | Oral Talk |  | A01254-MR | Monica Rodriguez     | QBIS-CAT, IQCC, Universitat de Girona  | CARBENE INSERTION TO Csp <sup>2</sup> -H BONDS CATALYZED BY A NON-HEME IRON COMPLEX   |
| S16 | Oral Talk |  | A01536-KO | Koji Oohora          | Osaka University   | Manganese Porphycene in a Myoglobin Matrix toward a Model of Cytochrome P450  |
| S16 | Oral Talk |  | A01781-SA | Santiago Alvarez     | Universitat de Barcelona   | Coordination spheres within proteins: a Shape analysis  |
| S16 | Oral Talk |  | A00215-XE | Xenia Engelmann      | German   | Synthesis, characterization and reactivity of high-valent transition metal-oxo complexes                                    |
| S16 | Oral Talk |  | A01282-GO | Giorgio Olivo        | Universitat de Girona  | Selective, Remote C-H Oxidation guided by Supramolecular Recognition  |
| S16 | Oral Talk |  | A00818-NM | Nadia Mosch-Zanetti  | Institute of Chemistry, University of Graz   | Mo and W Complexes for the Activation of O <sub>2</sub> and C <sub>2</sub> H <sub>2</sub> . Reactivity towards Lewis Acids  |
| S16 | Oral Talk |  | A02101-YM | Yuma Morimoto        | Osaka Univ.  | Characterization and Reactivities of a Bis(μ-oxido)dinickel(III) Complex with a Triplet Ground State                        |
| S16 | Oral Talk |  | A01580-PV | Praneeth Vijayendran | Institute for Molecular Science  | Redox Control of the Pentanuclear Iron Complexes by Ligand Modifications  |
| S16 | Oral Talk |  | A01958-YF | Yasuhiro Funahashi   | Department of Chemistry, Graduate School of Science, Osaka University                    | Dioxygen Activation on Distorted Dicopper Complexes Mimicking Type III Copper Proteins                                      |
| S16 | Oral Talk |  | A01646-TA | Tsukasa Abe          | Osaka University   | C-C Bond Formation Catalyzed by a Mononuclear Copper(II)-Superoxide Complex   |
| S16 | Oral Talk |  | A01161-SY | Syuhei Yamaguchi     | Ehime University   | Oxidation of Thioanisole with Hydrogen Peroxide over Copper(II)-Terpy Complexes Encapsulated in Zeolite                     |
| S16 | Oral Talk |  | A01005-TM | Tomoyo Misawa-Suzuki | Department of Materials and Life Sciences  | Conversion Reactions of Nitrate/Nitrite into Nitrogen Monoxide on the Doubly Oxido-Bridged Diruthenium Complexes            |
| S16 | Oral Talk |  | A01802-NP | Nanda Dulal Paul     | Department of Chemistry, Indian Institute of Engineering Science and Technology, Shibpur | Dehydrogenative Synthesis of Organo-heterocycles Using Transition Metal Complexes of Redox Noninnocent Azo-aromatic Pincers |
| S16 | Oral Talk |  | A01551-HK | Hiroaki Kotani       | University of Tsukuba  | Mechanistic insight into H-atom transfer reactions by Cr(V)-oxo complexes   |

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| S16 | Oral Talk |         | A01310-CC | Claraso Carlota     | QBIS-CAT, IQCC, Girona University  | Chiral Manganese Complexes with N4-Tetradentate Ligands as Catalysts for Epoxidation with Aqueous H <sub>2</sub> O <sub>2</sub>     |
| S16 | Oral Talk |         | A00699-YA | Yasuhiro Arikawa    | Graduate School of Engineering, Nagasaki University  | Synthetic Nitrite Reduction Cycle on a Dinuclear Ruthenium Complex Producing Ammonia  |
| S16 | Oral Talk |         | A01509-TT | Takehiko Tosha      | RIKEN SPring-8   | Elucidation of Mechanism of Biological Nitric Oxide Reduction   |
| S16 | Oral Talk |         | A01476-TW | Tohru Wada          | Rikkyo University  | Molecular Water Oxidation Catalysts with Deprotonatable Ligands   |
| S16 | Oral Talk |         | A00513-YY | Yasuyuki Yamada     | Research Center for Materials Science, Nagoya University                                     | Enhancement of Catalytic Ethane Oxidation Activity of $\mu$ -Nitride-Bridged Iron Porphyrinoid Dimer by Supramolecular Complexation |
| S16 | Oral Talk |         | A00882-SA | Shinya Ariyasu      | Nagoya University  | Catalytic Oxidation of Methane by Cytochrome P450BM3 Variants with Decoy Molecules  |
| S16 | Oral Talk |         | A01582-KO | Kei Ohkubo          | Osaka University   | Light-Driven Aerobic Oxygenation of Methane into Methanol and Formic Acid by Chlorine Dioxide                                       |
| S16 | Oral Talk |         | A01190-HS | Huatian Shi         | City University of Hong Kong   | Imido-Group Transfer of Activated Mn(V) Imido Tetraamido Macrocyclic Ligand Complex   |
| S16 | Poster    | July 31 | S16-P01   | Md Estak Ahmed      | Indian Association for the Cultivation of Science  | Role of Proton Relay in Bio-inspired Model Complexes Involved in H <sup>+</sup> and CO <sub>2</sub> Reduction                       |
| S16 | Poster    | July 31 | S16-P02   | Kana Nishikawa      | Nara Women's University  | Disproportionation of metal(IV) oxo complexes   |
| S16 | Poster    | July 31 | S16-P03   | Ikumi Terao         | Kanagawa Univ.   | Catalytic alkane oxidation activity of late 3d transition metal complexes with tris(oxazolylmethyl)amine ligand                     |
| S16 | Poster    | July 31 | S16-P04   | Laia Vicens         | QBIS-CAT, Institut de Quimica Computacional i Catalisi (IQCC), Universitat de Girona         | Combination of iron coordination compounds and peptides in bioinspired oxidation reactions: designing artificial enzymes            |
| S16 | Poster    | July 31 | S16-P05   | Michela Milan       | QBIS CAT, Institut de Quimica Computacional i Catalisi, University of Girona                 | Highly Enantioselective Oxidation of Non-activated Aliphatic C-H Bonds with Hydrogen Peroxide Catalyzed by Manganese Complexes      |
| S16 | Poster    | July 31 | S16-P06   | Santina Hoof        | Humboldt-Universitaet zu Berlin, Germany   | Trispyrazolylborato Metal(II) Flavonolate Complexes as models for the Quercetin Dioxygenase   |
| S16 | Poster    | July 31 | S16-P07   | Benjamin Herzigkeit | University of Kiel   | Small-molecule Model Systems of Tyrosinase: Synthetic and Spectroscopic Studies with various N-Donor Ligands                        |
| S16 | Poster    | July 31 | S16-P08   | Marco Cianfanelli   | Universitat de Girona  | The impact of diamine backbones on C-H oxidation catalyzed by Fe and Mn aminopyridine complexes                                     |
| S16 | Poster    | July 31 | S16-P09   | Valeria Dantignana  | QBIS, IQCC, Universitat de Girona  | Electronic effect in the formation and reactivity of [FeV(O)(O <sub>2</sub> CR)(L)] <sub>2</sub> <sup>+</sup>                       |
| S16 | Poster    | July 31 | S16-P10   | Yoshihiro Shimoyama | Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba | Formation and Reactivity of Ruthenium(III)-Oxyl Species Having an N-Heterocyclic Carbene Ligand                                     |
| S16 | Poster    | July 31 | S16-P11   | Toshiki Nishiura    | Kanagawa University  | Oxygen activation ability of mononuclear cobalt(II) complexes with N <sub>5</sub> donor sets and their reactivity.                  |