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|--------------------------|--|--|---|---|--|--|--|--|--|--|--|--|---|---|---|---|--|---|
|                          | A2-18  |  |   | A8-15   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 11:45 - 13:00            | <b>Lunch/Poster Session</b><br><i>(Location: LL4005 - 4107)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 13:00 - 14:30            | <b>Plenary Talk 5 -- Che Ting Chan, Hong Kong University of Science and Technology</b><br><b>Plenary Talk 6 -- Yuan Ping Feng, National University of Singapore</b><br><i>(Location: LL4001A-4103)</i>   |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 14:45 - 16:15            | <b>A2. Electronic Structure Methods and Their Applications</b>   | <b>A4. Modeling and Simulation of Nanoscale Spintronics Devices and Materials</b>      | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A8. Computational Chemistry</b>  | <b>B5. Quantum Computing</b>   | <b>A11. Electronic and Structural Responses of Materials to Electromagnetic Fields</b> | <b>A13. Computational Design of Energy Materials</b>           | <b>B4. Novel Superconductivity</b>                       | <b>B2. Quantum Many-Body Computation</b> | <b>C2. Kinetic Theory Based Numerical Schemes and Their Applications</b> | <b>C3. Numerical Simulation and Mathematical Modeling of Kinetic Equations</b> | <b>C7. Novel Computational Techniques for Photonics</b>                        | <b>C8. Mathematical and Computational Problems in Quantum Systems</b> | <b>C9. Recent Development of High Order Numerical Methods for Hyperbolic Conservation Laws and Its Applications</b> | <b>C11. Recent Advances in Numerical Methods to PDEs with Multiscale and/or Random Coefficients</b> | <b>C13. Mini-Symposium on Adaptive Methods and Acceleration Techniques in Numerical Simulations</b>                 | <b>D6. Water, Ice, and Aqueous Solutions</b> | <b>C16. Modeling and Computations in Big Data</b>                           |
|                          | A2-4   | A4-13  | A6-14   | A8-16   | B5-9   | A11-15   | A13-13   | B4-1   | B2-7                                     | C2-13  | C3-4   | C7-4   | C8-13   | C9-10   | C11-10  | C13-10  | D6-10  | C16-4   |
|                          | A2-5   | A4-14  | A6-15   | A8-17   | B5-10  | A11-16   | A13-14   | B4-2   | B2-8                                     | C2-14  | C3-5   | C7-5   | C8-14   | C9-11   | C11-11  | C13-11  | D6-11  | C16-5   |
|                          | A2-6   | A4-15  | A6-16   | A8-18   | B5-11  | A11-17   | A13-15   | B4-3   | B2-9                                     | C2-15  | C3-6   | C7-6   | C8-15   | C9-12   |   | C13-12  | D6-12  | C16-6   |
|                          |  |  |   |   |  |  |  |  |  | C2-34  |  | C7-7   |   |   |   |   |  |   |
|                          |  |  |   |   |  |  |  |  |  |  |  | C7-8   |   |   |   |   |  |   |
| 16:15 - 16:30            | <b>Coffee Break</b><br><i>(Location: Foyer 4 F)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 16:30 - 18:30            | <b>A2. Electronic Structure Methods and Their Applications</b>   | <b>A6. Computational Study on Nanoscale Materials</b>                                  | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A8. Computational Chemistry</b>  | <b>A9. Heat Transport in Nanostructures and Functional Materials</b> | <b>A11. Electronic and Structural Responses of Materials to Electromagnetic Fields</b> | <b>A13. Computational Design of Energy Materials</b>           | <b>B4. Novel Superconductivity</b>                       | <b>B2. Quantum Many-Body Computation</b> | <b>C2. Kinetic Theory Based Numerical Schemes and Their Applications</b> | <b>C4. Numerical Methods of Nonlinear Problems</b>                             | <b>C14. Numerical Methods for Stochastic Differential Equations</b>            | <b>C8. Mathematical and Computational Problems in Quantum Systems</b> | <b>C9. Recent Development of High Order Numerical Methods for Hyperbolic Conservation Laws and Its Applications</b> |   | <b>D3. Computational Inverse Problems in Physics and Biomedicine</b>  | <b>D6. Water, Ice, and Aqueous Solutions</b> | <b>D1. Mini-Symposium on Computational Pharmaceutics</b>                    |
|                          | A2-7   | A6-17  | A6-21   | A8-19   | A9-1   |  | A13-16   | B4-4   | B2-10                                    | C2-16  | C4-7   | C14-3  | C8-16   | C9-13   |   | D3-4  | D6-13  | D1-4  |
|                          | A2-8   | A6-18  | A6-22   | A8-20   | A9-2   | A11-18   | A13-17   | B4-5   | B2-11                                    | C2-17  | C4-9   | C14-4  | C8-17   | C9-14   |   | D3-5  | D6-14  | D1-5  |
|                          | A2-9   | A6-19  | A6-23   | A8-21   | A9-3   | A11-19   | A13-18   | B4-6   | B2-12                                    | C2-18  | C4-13  | C14  | C8-18   | C9-15   |   | D3-6  | D6-15  | D1-6  |
| A2-16                    | A6-20  | A6-24  | A8-22   |   |  | A13-19   |  |  | C2-23                                    |  | C14  |  |   |   |   |   |  |   |
| <b>19 Jan 2017 (Thu)</b> |  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| Time                     | TF4202   | TF4203   | TF4204  | TF4205  | TF4201A  | TF4206   | TF4207   | TF4201B  | TF4302                                   | TF4303   | TF4304   | TF4305   | TF4306  | TF4307  | TF4301A   | LL4104  | LL4004                                       | TF4301B   |
| 08:00 - 17:00            | <b>On-Site Registration</b><br><i>(Location: Foyer 4 F)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 08:30 - 10:00            |  |  |   |   |  | <b>A11. Electronic and Structural Responses of Materials to Electromagnetic Fields</b> |  |  |  |  |  |  |   |   |   |   |  |   |
|                          |  |  |   |   |  | A11-20   |  |  |  |  |  |  |   |   |   |   |  |   |
|                          |  |  |   |   |  | A11-21   |  |  |  |  |  |  |   |   |   |   |  |   |
|                          |  |  |   |   |  | A11-22   |  |  |  |  |  |  |   |   |   |   |  |   |
| 10:00 - 10:15            | <b>Coffee Break</b><br><i>(Location: Foyer 4 F)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 10:15 - 11:45            | <b>A2. Electronic Structure Methods and Their Applications</b>   | <b>D4. Modeling and Simulation of Macromolecular Systems: Methods and Applications</b> | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A7. High Pressure Physics as a Tool to Design New Functional Materials</b> | <b>A9. Heat Transport in Nanostructures and Functional Materials</b> | <b>A11. Electronic and Structural Responses of Materials to Electromagnetic Fields</b> | <b>A12. Excited State Dynamics in Condensed Matter Physics</b> | <b>D1. Mini-Symposium on Computational Pharmaceutics</b> | <b>B2. Quantum Many-Body Computation</b> | <b>C2. Kinetic Theory Based Numerical Schemes and Their Applications</b> | <b>C4. Numerical Methods of Nonlinear Problems</b>                             | <b>C14. Numerical Methods for Stochastic Differential Equations</b>            | <b>C8. Mathematical and Computational Problems in Quantum Systems</b> | <b>C10. PDE Based Image Processing Techniques and Their Applications</b>  | <b>C12. Software Platforms and Libraries for Computational Physics</b>                              | <b>C13. Mini-Symposium on Adaptive Methods and Acceleration Techniques in Numerical Simulations</b>                 | <b>D6. Water, Ice, and Aqueous Solutions</b> | <b>B1. Modeling Quantum Transport at Nanoscale</b>                          |
|                          | A2-10  | D4-6   | A6-25   | A7-1  | A9-4   | A11-23   | A12-4  | D1-7   | B2-13                                    | C2-10  | C4-10  | C14-5  | C8-19   | C10-4   | C12-1   | C13-13  | D6-16  | B1-7  |
|                          | A2-11  | D4-8   | A6-26   | A7-2  | A9-5   | A11-24   | A12-5  | D1-8   | B2-14                                    | C2-20  | C4-10  | C14-6  | C8-20   | C10-5   | C12-2   | C13-14  | D6-17  | B1-8  |
|                          | A2-12  | D4-9   | A6-27   | A7-3  | A9-6   | A11-25   | A12-6  | D1-9   | B2-15                                    | C2-21  | C4-11  | C14-7  | C8-21   | C10-6   | C12-3   | C13-15  | D6-18  | B1-9  |
| A2-19                    | D4-10  |  |   |   |  |  |  |  | C2-24                                    |  | C14-8  |  |   |   |   |   |  | B1-10   |
| A2-20                    |  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 11:45 - 13:00            | <b>Lunch/Poster Session</b><br><i>(Location: LL4005 - 4107)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 13:00 - 14:00            | <b>Plenary Talk 9 -- Robert A. DiStasio, Cornell University, Department of Chemistry and Chemical Biology</b><br><b>Plenary Talk 10 -- Hui Pan, Institute of Applied Physics and Materials Engineering, University of Macau</b><br><i>(Location: LL4001A-4103)</i> |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 14:00 - 15:30            | <b>A2. Electronic Structure Methods and Their Applications</b>   |  | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A8. Computational Chemistry</b>  | <b>A9. Heat Transport in Nanostructures and Functional Materials</b> | <b>B3. Lattice Quantum Chromodynamics</b>  | <b>A12. Excited State Dynamics in Condensed Matter Physics</b> |  | <b>B2. Quantum Many-Body Computation</b> | <b>C2. Kinetic Theory Based Numerical Schemes and Their Applications</b> | <b>C6. High-Order Methods and Their Applications in Computational Physics</b>  | <b>C14. Numerical Methods for Stochastic Differential Equations</b>            | <b>C8. Mathematical and Computational Problems in Quantum Systems</b> | <b>C10. PDE Based Image Processing Techniques and Their Applications</b>  | <b>C12. Software Platforms and Libraries for Computational Physics</b>                              | <b>C13. Mini-Symposium on Adaptive Methods and Acceleration Techniques in Numerical Simulations</b>                 | <b>D6. Water, Ice, and Aqueous Solutions</b> | <b>D5. Modeling and Computation for Biophysical and Soft Matter Systems</b> |
|                          | A2-13  |  | A6-28   | A8-23   | A9-7   | B3-1   | A12-7  |  | B2-16                                    | C2-25  | C6-7   | C14-9  | C8-22   | C10-7   | C12-4   | C13-16  | D6-19  | D5-4  |
|                          | A2-14  |  | A6-29   | A8-24   | A9-8   | B3-2   | A12-8  |  | B2-17                                    | C2-26  | C6-8   | C14  | C8-23   | C10-8   | C12-5   | C13-17  | D6-20  | D5-2  |
|                          | A2-15  |  | A6-30   | A8-25   | A9-9   | B3-3   | A12-9  |  | B2-18                                    | C2-27  | C6-9   | C14  | C8-24   | C10-9   | C12-6   |   | D6-21  | D5-3  |
|                          |  |  | A8-26   |   |  |  |  |  |  |  |  | C14  |   |   |   |   |  |   |
|                          |  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
|                          |  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 15:30 - 15:45            | <b>Coffee Break</b><br><i>(Location: Foyer 4 F)</i>  |  |   |   |  |  |  |  |  |  |  |  |   |   |   |   |  |   |
| 15:45 - 17:45            | <b>A1. Computational Methods for Low-dimensional Materials</b>   | <b>A4. Modeling and Simulation of Nanoscale Spintronics Devices and Materials</b>      | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A7. High Pressure Physics as a Tool to Design New Functional Materials</b> | <b>A9. Heat Transport in Nanostructures and Functional Materials</b> | <b>B3. Lattice Quantum Chromodynamics</b>  | <b>A12. Excited State Dynamics in Condensed Matter Physics</b> | <b>B4. Novel Superconductivity</b>                       | <b>B2. Quantum Many-Body Computation</b> | <b>C2. Kinetic Theory Based Numerical Schemes and Their Applications</b> | <b>C6. High-Order Methods and Their Applications in Computational Physics</b>  | <b>C3. Numerical Simulation and Mathematical Modeling of Kinetic Equations</b> |   | <b>C10. PDE Based Image Processing Techniques and Their Applications</b>  | <b>C5. Mathematical Analysis of Plasmonic Resonance and Related Topics</b>                          | <b>C9. Recent Development of High Order Numerical Methods for Hyperbolic Conservation Laws and Its Applications</b> | <b>D6. Water, Ice, and Aqueous Solutions</b> | <b>D5. Modeling and Computation for Biophysical and Soft Matter Systems</b> |
|                          | A1-1   | A4-16  | A6-31   | A7-4  | A9-10  | B3-4   | A12-10   | B4-7   | B2-19                                    | C2-28  | C6-10  | C3-7   |   | C10-10  | C5-1  | C9-16   | D6-22  | D5-4  |
|                          | A1-2   | A4-17  | A6-32   | A7-5  | A9-11  | B3-5   | A12-11   | B4-8   | B2-20                                    | C2-29  | C6-11  | C3-8   |   | C10-11  | C5-2  | C9-17   | D6-23  | D5-5  |
|                          | A1-3   | A4-18  | A6-33   | A7-6  | A9-12  | B3-6   | A12-12   | B4-9   | B2-21                                    | C2-30  | C6-12  | C3-9   |   | C10-12  | C5-3  | C9-18   | D6-24  | D5-6  |
| A1-4                     | A4-19  | A6-34  | A7-7  | A9-13   | B3-7   | A12-13   | B4-10  | B2-22  |  |  | C3-10  |  | C10-13  | C5-4  | C9-19   | D6-25   | D5-7   |   |

|                          |   |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
|--------------------------|---|---|---|------------------------------------|--|---|--------|--|--|--|--------|--------|--|--|--|--------|--------|---|
| 19:00 - 21:30            | <b>Banquet</b><br><b>Best Paper Awards Presentation</b><br><i>(Location: The Landmark Macau)</i>  |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
| <b>20 Jan 2017 (Fri)</b> |   |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
| Time                     | TF4202  | TF4203  | TF4204  | TF4205                             | TF4201A  | TF4206                                    | TF4207 | TF4201B  | TF4302   | TF4303   | TF4304 | TF4305 | TF4306   | TF4307   | TF4301A  | LL4104 | LL4004 | TF4301B   |
| 08:00 - 09:00            | <b>On-Site Registration</b><br><i>(Location: Foyer 4 F)</i>   |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
| 08:45 - 09:45            | <b>Public Lecture II -- Aaron Ciechanover, 2004 Nobel laureate in Chemistry, The Technion - Israel Institute of Technology</b><br><i>(Location: LL4001A-4103)</i> |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
| 09:45 - 10:00            | <b>Coffee Break</b><br><i>(Location: Foyer 4 F)</i>   |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |
| 10:00 - 12:00            | <b>B2. Quantum Many-Body Computation</b>  | <b>A4. Modeling and Simulation of Nanoscale Spintronics Devices and Materials</b> | <b>A6. Computational Study on Nanoscale Materials</b> | <b>A8. Computational Chemistry</b> | <b>A1. Computational Methods for Low-dimensional Materials</b> | <b>B3. Lattice Quantum Chromodynamics</b> |        | <b>C1. Computation and Visualization of Fluid Flow and Heat Transfer</b> | <b>C3. Numerical Simulation and Mathematical Modeling of Kinetic Equations</b> | <b>C4. Numerical Methods of Nonlinear Problems</b> |        |        | <b>C12. Software Platforms and Libraries for Computational Physics</b> | <b>D3. Computational Inverse Problems in Physics and Biomedicine</b> | <b>C5. Mathematical Analysis of Plasmonic Resonance and Related Topics</b> |        |        | <b>D5. Modeling and Computation for Biophysical and Soft Matter Systems</b> |
|                          | B2-23   | A4-20   | A6-35   | A8-27                              | A1-5   | B3-8                                      |        | C1-1   | C3-11  | C4-12  |        |        | C12-7  | D3-7   | C5-5   |        |        | D5-8  |
|                          | B2-24   | A4-21   | A6-36   | A8-28                              | A1-6   | B3-9                                      |        | C1-2   | C3-12  | C4-12  |        |        | C12-8  | D3-8   | C5-6   |        |        | D5-9  |
|                          | B2-25   | A4-22   | A6-37   | A8-29                              | A1-7   | B3-10                                     |        | C1-3   | C3-13  | C4-12  |        |        | C12-9  | D3-9   | C5-7   |        |        | D5-10   |
|                          | B2-26   | A4-23   | A6-38   | A8-30                              |  | B3-11                                     |        | C1-4   | C3-14  | C4-15  |        |        | C12-10   | D3-10  |  |        |        | D5-11   |
|                          |   |   | A6-39   | A8-31                              |  | B3-12                                     |        | C1-5   | C3-15  |  |        |        |  | D3-11  |  |        |        | D5-12   |
|                          |   |   | A6-40   |                                    |  |   |        | C1-6   | C3-16  |  |        |        |  | D3-12  |  |        |        | D5-13   |
|                          |   |   | A6-41   |                                    |  |   |        | C1-7   |  |  |        |        |  | D3-13  |  |        |        |   |
|                          |   |   | A6-42   |                                    |  |   |        | C1-8   |  |  |        |        |  | D3-14  |  |        |        |   |
|                          |   |   | A6-43   |                                    |  |   |        |  |  |  |        |        |  | D3-15  |  |        |        |   |
|                          |   | A6-44   |   |                                    |  |   |        |  |  |  |        |        | D3-16  |  |  |        |        |   |
|                          |   |   |   |                                    |  |   |        |  |  |  |        |        | D3-17  |  |  |        |        |   |
| 12:00 - 13:30            | <b>Lunch</b><br><i>(Location: LL4005 - 4107)</i>  |   |   |                                    |  |   |        |  |  |  |        |        |  |  |  |        |        |   |