

HANAMI HIGH-LEVEL SYMPOSIUM

2ND EDITION

AGENDA

Materials Science Session

December 10, Wednesday

Morning Session

Chair: Giacomo Giorgi

9:00 AM

Opening Remarks

9:05 AM

Tensor Networks in the age of machine learning | **Xavier Waintal**

9:30 AM

Data-driven kinetic energy functionals for orbital-free DFT: from ML to formulae | **Sergei Manzhos** | Online

9:55 AM

EU-Japan Collaborations on Materials Science - AI and HPC | **William Dawson**

10:20 AM

Impact of MxP on Dense Eigenvalue Computation | **Toshiyuki Imamura**

10:45 AM

Coffee Break

11:05 AM

ChASE: advancing a modern GPU-distributed eigensolver library for applications in Materials Science | **Edoardo Di Napoli**



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11:30 AM

Expanding ChASE to solve for pseudo-hermitian Hamiltonians with applications to excitonic physics | **Clement Richefort**

11:55 AM

Lessons learned from the cross-platform porting of the BigDFT's Poisson solver | **David Amblard**

12:20 PM

From Large-Scale DFT to a New Research Paradigm: The Complexity-Reduction Framework in BigDFT | **Luigi Genovese**

13:00 PM

Lunch

Afternoon Session

Chair: Edoardo Di Napoli

02:30 PM

Preventing lead leakage in perovskite solar cells with a sustainable titanium dioxide sponge | **Giuseppe Fisicaro**

02:55 PM

Protective Role of Germania on (Sn,Ge)-Mixed Halide Perovskites | **Giacomo Giorgi**

03:20 PM

Coffee Break

03:30 PM

Scientific Advisory Board

07:30 PM

Networking Dinner

December 11, Thursday

Morning Session

Chair: Daniele Varsano

9:00 AM

First-principles calculations for dephasing effects in laser-solid interactions | **Kazuhiro Yabana**

9:25 AM

Transformations and transport processes in the solid state: Static and dynamic aspects | **Stefano Leoni**

9:50 AM

Electronic Transport in Two-dimensional Materials | **Alessandro Pecchia**

10:15 AM

Towards a NEGF-Compatible Excitonic Self-Energy | **Flavia Carafone**

10:40 AM

Coffee Break

11:00 AM

All-Electron GW and Bethe-Salpeter Calculations for Complex Systems | **Ivan Duchemin**

11:25 AM

Ab initio many-body perturbation theory towards the exascale: Yambo on GPUs | **Andrea Ferretti**

11:50 AM

Short Conclusion Plenary

12:15 AM

Lunch and Departure



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