

## **Session Program**

**28-31 Aug 2018**



## **Annual meeting of the Swiss Physical Society 2018**

### ***Advanced Electronic-Structure Developments and Applications***

EPFL

# Wednesday 29 August

16:30

## Advanced Electronic-Structure Developments and Applications: I

Session | Location: EPFL, CE 2

16:30–17:00

**【501】 Electronic structures through \$GW\$ and hybrid functionals: from defect levels to band gaps**

**Speaker**

Dr Wei Chen

17:00–17:15

**【502】 Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic**

**Speaker**

Dr Nicola Colonna

17:15–17:30

**【503】 Electronic structure and excitonic effects in the photoanode  $\beta$ -Cu<sub>2</sub>V<sub>2</sub>O<sub>7</sub>**

**Speaker**

Igor Reshetnyak

17:30–17:45

**【504】 pH-dependent surface chemistry and catalytic reaction pathway from first-principles**

**Speaker**

Dr Francesco Ambrosio

17:45–18:00

**【505】 Transition-metal compounds from extended Hubbard functionals**

**Speaker**

Matteo Cococcioni

18:00–18:15

**【506】 Hubbard interactions from density-functional perturbation theory**

**Speaker**

Iurii Timrov

18:15

# Thursday 30 August

17:00

## Advanced Electronic-Structure Developments and Applications: II

Session | Location: EPFL, CE 2

17:00–17:30

**【511】 Nonempirical hybrid functionals unravel the intricate mechanisms of self-compensation in Mg-doped GaN**

**Speaker**

Giacomo Miceli

17:30–17:45

**【512】 Quantitative modelling of Pt(111)/water interface under bias potential through constant Fermi-level molecular dynamics**

**Speaker**

Assil Bouzid

17:45–18:00

**【513】 Surface Polarons Reducing the Overpotentials in the Oxygen Evolution Reaction**

**Speaker**

Patrick Gono

18:00–18:15

**【514】 First-principles-based prediction of yield strength in the RhIrNiPdPtCu high entropy alloy**

**Speaker**

Dr Binglun Yin

18:15–18:30

**【515】 Silicon liquid structure and crystal nucleation from ab-initio deep metadynamics**

**Speaker**

Luigi Bonati

18:30–18:45

**【516】 Ordering at the Ga/GaAs interface. Combining first-principles and machine-learning simulations**

**Speaker**

Mr Giulio Imbalzano

18:45