

Workshop on
“Polarons in the 21st Century”

December 9 –13, 2019

organized by

Jozef Devreese (U Antwerpen), Cesare Franchini (U Vienna), Georg Kresse (U Vienna), Jacques Tempere (U Antwerpen)

• **Monday, December 9th, 2019**

09:00 – 09:20 **Registration**

09:20 – 09:40 **Welcome and Opening**

09:40 – 10:40 **Jacques Tempere (U Antwerpen)**

Polaron physics through the XX and XXI centuries

10:40 – 11:20 **Aaron Deskins (Worcester Polytechnic Institute)**

Strategies for Modeling Polarons using Electronic Structure Methods

11:20 – 11:50 **Coffee / Tea Break**

11:50 – 12:30 **Joannis Koepsell (MPG Munich)**

New perspective on magnetic polarons in antiferromagnetic Mott insulators from cold atoms

12:30 – 14:00 **Lunch Break**

14:00 – 14:40 **Christof Wöll (KIT, Karlsruhe)**

Polarons on Oxides Detected by Infrared-Reflection Absorption Spectroscopy (IRRAS): The Case of TiO_2 and ZnO

14:40 – 15:00 **Frank Ortmann (TU Dresden)**

Vibrations and their Impact on Electronic and Transport Properties of Organic Materials

15:00 – 15:30 **Coffee / Tea Break**

15:30 – 16:10 **Stephan Lany (NREL, Golden)**

Direct first-principles calculation of polarons in Koopmans-corrected DFT

16:10 – 16:30 **Iflah Laraib (U Delaware)**

Electronic structure of $YTiO_3$ and the charge transport through small polaron hopping

• **Tuesday, December 10th, 2019**

09:00 – 09:40 **Feliciano Giustino (U of Texas, Austin)**

Looking inside a polaron

09:40 – 10:20 **Thomas Hahn (U Vienna) & Manuel Engel (U Vienna)**

Diagrammatic Monte Carlo for Polarons from First Principles

10:20 – 11:00 **Coffee / Tea Break**

11:00 – 11:40 **Jarvist Moore Frost (Imperial College, London)**

Polaron mobility and response functions in the Feynman variational approximation

- 11:40 – 12:20 **Alison Walker (U Bath)**
Multi scale modelling of organic devices and perovskite solar cells
- 12:20 – 14:00 **Lunch Break**
- 14:00 – 14:40 **Mikhail Lemeshko (ISTA, Klosterneuburg)**
Quasiparticle approach to molecules rotating in quantum solvents
- 14:40 – 15:00 **Giacomo Bighin (ISTA, Klosterneuburg)**
Diagrammatic Monte Carlo approach to angular momentum in quantum many-body systems
- 15:00 – 15:30 **Coffee / Tea Break**
- 15:30 – 16:10 **Marco Grioni (EPFL Lausanne)**
ARPES signatures of polarons
- 16:10 – 16:30 **Carla Verdi (U Vienna)**
Polaronic satellites in angle-resolved photoemission spectra from ab initio many-body calculations
- 16:55 – 19:00 **Poster Session**
- 17:00 – 19:00 **Akash Singh (IIS Bengaluru)**
Engineering Defect Transition-Levels through van der Waals Heterostructure
- 17:00 – 19:00 **Ji Chen (Peking U)**
Interplay between small polarons and water on TiO_2 surfaces
- 17:00 – 19:00 **Thomas Hahn (U Vienna)**
Diagrammatic Monte Carlo for Polarons from First Principles
- 17:00 – 19:00 **Weng Hong Sio (U Oxford)**
Two-dimensional polarons: the case of monolayer BN
- 17:00 – 19:00 **Igor Sokolović (TU Vienna)**
Interactions of O_2 and CO molecules with small electronic polarons on the TiO_2 (110) surface
- 17:00 – 19:00 **Matthias Meier (TU Vienna)**
Polarons in Fe_2O_3 : Affecting H_2O Diffusion and Desorption
- 17:00 – 19:00 **Timour Ichmoukhamedov (U Antwerpen)**
(poster) Feynman path-integral treatment of the Bose polaron beyond the Fröhlich model
- 17:00 – 19:00 **Juraj Krsnik (IFS, Zagreb)**
Electron scattering and bound states in the presence of polaronic impurities
- 17:00 – 19:00 **Matthew Houtput (U Antwerpen)**
Beyond-Fröhlich Hamiltonian for large polarons in anharmonic solids (Poster presentation)
- 17:00 – 19:00 **Manuel Engel (U Vienna)**
Electron-Phonon Interactions using the Projector-Augmented-Wave Method
- 17:00 – 19:00 **Sabine Körbel (Trinity College, Dublin)**
Polarons at ferroelectric domain walls in $BiFeO_3$
- 17:00 – 19:00 **Supriti Ghorui (IIT, Bombay)**
Optoelectronic Properties and Defect Physics of Lead-free Photovoltaic Absorbers $Cs_2Au^{(I)}Au^{(III)}X_6$ ($X = I, Br$)
- 17:00 – 19:00 **Jiban Kangsabanik (IIT Bombay)**
Lattice Dynamics and Electron-phonon coupling in Lead free Bi^{3+} Alloyed $Cs_2AgInCl_6$ Double Perovskite Nanocrystals
- 17:00 – 19:00 **Luis Ardila (ITP Hannover)**
POSTER: From polarons to bipolarons in Bose-Einstein condensates.

• **Wednesday, December 11th, 2019**

09:00 – 09:40 **Robert Seiringer (ISTA, Klosterneuburg)**

The Fröhlich polaron at strong coupling

09:40 – 10:20 **Sergio Ciuchi (U LAquila)**

Disorder-induced polarons in strongly disordered metals (and doped oxides)

10:20 – 11:00 **Coffee / Tea Break**

11:00 – 11:40 **Alexander Shluger (University College London)**

Polarons and intrinsic electron and hole trapping in amorphous oxides

11:40 – 12:20 **Cristiana Di Valentin (U Milano-Bicocca)**

Polaronic effects in titanium and iron oxides by hybrid density functional theory calculations.

12:20 – 14:00 **Lunch Break**

14:00 – 14:40 **Xiaoyang Zhu (Columbia University, New York)**

Ferroelectric Polarons and Belgian Waffles in Lead Halide Perovskites

14:40 – 15:00 **Julia Wiktor (CUT, Göteborg)**

Polarons in photoabsorbing materials: Role in solar cells and water-splitting devices

15:00 – 15:30 **Coffee / Tea Break**

15:30 – 16:10 **Richard Schmidt (MPI Quantum Optics, Garching)**

Polaronic effects in condensed matter and atomic systems

16:10 – 16:30 **Felix Rose (MPI Quantum Optics, Garching)**

Disorder in order: simulating a random scattering potential with a randomless cold atom system

19:00 – 22:00 **Social Dinner**

• **Thursday, December 12th, 2019**

09:00 – 09:40 **Elio Giamello (U Torino)**

Charge carriers trapping in semiconducting metal oxides. The point of view of an EPR spectroscopist.

09:40 – 10:20 **Chris Van de Walle (UC, Santa Barbara)**

Impact of small polarons on the properties of transition-metal oxides

10:20 – 11:00 **Coffee / Tea Break**

11:00 – 11:40 **Frédéric Chevy (ENS Paris)**

The $2N+1$ body problem: An impurity immersed in a strongly correlated fermionic superfluid

11:40 – 12:20 **Jan Arlt (U Aarhus)**

Universal dynamics of impurities in a Bose-Einstein condensate

12:20 – 14:00 **Lunch Break**

14:00 – 14:40 **Martin Setvin (TU Vienna)**

Combined STM/AFM: Watching polarons at the atomic level

14:40 – 15:00 **Xavier Gonze (UCLouvain)**

Dynamical effects in zero-point renormalization of the band gap: connecting first-principles approach and Fröhlich model

15:00 – 15:30 **Coffee / Tea Break**

15:30 – 16:10 **Annabella Selloni (Princeton U)**

Localized and Delocalized Excess Electrons States in Reduced Anatase TiO_2

16:10 – 16:30 **Matthew Wolf (U Bath)**

Band-Electron vs. Polaron Mobility in Metal-Halide Perovskites

- **Friday, December 13th, 2019**

09:00 – 09:40 **Serghei Klimin (U Antwerpen)**

Equilibrium and response properties of a many-polaron gas

09:40 – 10:20 **Michele Reticcioli (U Vienna)**

Intrinsic polaron formation and influence on the surface chemical properties

10:20 – 11:00 **Coffee / Tea Break**

11:00 – 11:40 **Sebastian Kokott (FHI der MPG Berlin)**

Simulating Small Polarons from First Principles: The DFT supercell approach

11:40 – 12:00 **Patrick Gono (EPFL Lausanne)**

Surface Polarons Reducing Overpotentials in the Oxygen Evolution Reaction

All talks take place at ESI Boltzmann Lecture Hall!