



## On-line Workshop on Excited Charge Dynamics in Semiconductors | (SMR 3516)

28 Sep 2020 - 30 Sep 2020  
Virtual, Virtual

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### **P01 - ADANE Getie Tsigie**

Electronic Properties of 2D Van der Waals Heterostructures of Janus Transition Metal Dichalcogenides with WS<sub>2</sub> Monolayer for Photovoltaic Devices: A First Principle study

### **P02 - BAYAWA Mohamed**

Calculation of Exciton Energies and Lifetimes for Solar Cell Modeling using the Density Functional Theory (DFT) and the Bethe-Salpeter Equation (BSE).

### **P03 - FANKAM FANKAM Jean Baptiste**

Theoretical investigation of the molecular structure, vibrational spectra, thermodynamic and nonlinear optical properties of 4, 5-dibromo-2, 7-dinitro- fluorescein

### **P04 - FOBASSO MBOGNOU Florette Corinne**

Stability of an excitonic in an extrinsic semiconductor

### **P05 - KENFACK Sadem Christian**

properties of polaron in monolayer graphene under laser field

### **P06 - MANYALI Simiyu George**

First-principles calculation on electron transport properties of carbon nitride

### **P07 - NAGURA Langson Jonah**

First Principles investigations of electron-hole inclusion effects on optoelectronic properties of HgInTe<sub>4</sub>

### **P08 - OYENIYI Ezekiel**

Semi-empirical Model from high-level ab-initio data for the calculation of Excitation Energies and Absorption spectra for Cu, Ag, and Ag-Cu Bimetallic Nanoclusters

### **P09 - AFSANEH Elaheh**

Entanglement formation between a semiconductor quantum dot molecule including phonon interactions

### **P10 - BASERA Pooja**

Role of defects in MAPbI<sub>3</sub> to modulate optical absorption and solar cell efficiency

### **P11 - BHAGAT Rajesh Brajesh**

Effective charge separation in Ag-loaded and P-doped tri-s-triazine C<sub>3</sub>N<sub>4</sub> single-layer for efficient H<sub>2</sub> evolution

### **P12 - CHANDRA Swarniv**

Electron-Acoustic Waves in electron- hole semiconductor plasma

### **P13 - CHEN Ji**

Interplay between small polarons and water on TiO<sub>2</sub> surfaces

### **P14 - DEBATA Suryakanti**

Structural, optical and charge transport properties of ring-fused PDI-dimers

### **P15 - DEB Jyotirmoy**

Boron-nitride and boron-phosphide doped twin-graphene: Applications in electronics and optoelectronics

**P16 - DIN Haleem Ud**

Rashba spin splitting and photocatalytic properties of GeC – M SSe ( M = Mo , W) van der Waals heterostructures

**P17 - GHOSH Dibyajyoti**

Charge Carrier Dynamics in Layered Halide Perovskites: A Computational Insights

**P18 - KARMAKAR Manobina**

Exciton dynamics in MoS<sub>2</sub> under below-resonance ultrafast photo-excitation

**P19 - KHATIBI Zahra**

Dynamics of Exciton condensate in a topological one-dimensional model

**P20 - KUMAR Manish**

Role of Defects in Photocatalytic Water Splitting: Monodoped vs Codoped SrTiO<sub>3</sub>

**P21 - MISHRA Bhusan Shashi**

Design and Electronic Structure Analysis of Graphene/Anatase TiO<sub>2</sub> (001) Interface

**P22 - PENG Bo**

Topological phonons in oxide perovskites controlled by light

**P23 - QUEK Su Ying**

Quasiparticle levels at large interface systems from many-body perturbation theory: the XAF-GW method

**P24 - SARKAR Utpal**

Exploring the carrier mobility of pentagraphene

**P25 - SINHA Sapna**

Direct Laser Patterning and Phase Transformation of 2D PdSe<sub>2</sub> Films for On-Demand Device Fabrication

**P26 - WANG Juefan**

Isolated Flat Bands and Physics of Mixed Dimensions in a 2D Covalent Organic Framework

**P27 - XUAN Fengyuan**

Valley Zeeman effect and Landau levels in two-dimensional transition metal dichalcogenides from many-body perturbation theory

**P28 - ZIASHAHABI Azin**

optical properties of rutile TiO<sub>2</sub> nanoparticles with different concentration of oxygen defects

**P29 - ALVERTIS Markos Antonios**

Impact of exciton delocalization on exciton-vibration interactions in organic semiconductors

**P30 - BRUNIN René François Guillaume**

Electron-Phonon Beyond Fröhlich: Dynamical Quadrupoles in Polar and Covalent Solids

**P31 - DIEZ CABANES Valentin**

Why mixed halide perovskites do (or not) work? A static and dynamic analysis

**P33 - FROST Moore Jarvist**

Mobility, Defect Scattering, Vibrational Response of Feynman Polarons in Halide Perovskites

**P34 - GIANNINI Samuele**

Flickering Polarons Mediate Charge Transport in Organic Semiconducting Crystals

**P35 - JANKOVIĆ Veljko**

Energy-Temporal Pathways of Free-Charge Formation at Organic Bilayers: Competition of Delocalization, Disorder, and Polaronic Effects

**P36 - KNIPPENBERG Stefan**

Multiscale modeling of conjugated probes embedded in lipid bilayer membranes

**P37 - KOERBEL Margrit Sabine**

Polarons at ferroelectric domain walls in BiFeO<sub>3</sub>

**P38 - MARSILI Margherita**

"Real time electronic dynamics of molecules close to a plasmonic nanoparticle: combining GW-BSE, and PCM approaches"

**P39 - MARTSINOVICH Natalia**

Graphene-based materials as electrochemical sensors

**P40 - RIVERA Miguel**

Software Solutions for Charge Hopping Rates in the Marcus Regime

**P41 - SPONZA Lorenzo**

Changes of the optical gap due to environmental screening in 2D black phosphorus

**P42 - TAL Aleksei**

Accurate optical spectra through time-dependent density functional theory based on screening-dependent hybrid functionals

**P43 - VANZAN Mirko**

Computational insight on the energy transfer properties of small noble metal nanoclusters

**P44 - BUSTAMANTE Mauricio Carlos**

Radiative Decay in Real-Time Electron Dynamics

**P45 - CABELLOS QUIROZ Jose Luis**

Optical spin injection on graphane, silicene, and SiC monolayers.

**P46 - GADEA David Esteban**

Radiative Decay in Real-Time Electron Dynamics