Defects in Two-dimensional Materials

750. WE-Heraeus-Seminar

08 May - 12 May 2023

at the Physikzentrum Bad Honnef, Germany

WILHELM UND ELSE
HERAEUS-STIFTUNG

Program

Sunday, 7 May 2023

17:00 – 21:00	Registration	
From 18:00	*BUFFET SUPPER and informal get-together*	

Monday, 8 May 2023

08:00	*BREAKFAST*	

Chair: Stefan Facsko

09:00 – 09:15	Scientific organizers	**Welcome words**
09:15 – 09:45	Arkady Krasheninnikov	**Introduction: What is special about defects in 2D materials?**
09:45 – 10:30	Matthias Batzill	**Excess Metal Induced Defect Formation and Compositional Phase Transformations in 2D Transition Metal Dichalcogenides**
10:30 – 10:50	Herve Aubin	**Hydrogenic Spin-Valley states in Bromine-doped 2H-MoTe2**
10:50 – 11:30	*COFFEE BREAK*	

Chair: Andrey Turchanin

11:30 – 12:15	Kristian Thygesen	**How ab initio calculations can help identifying useful defects for quantum technology**
12:15 – 12:35	Harriet Åhlgren	**Introducing individual metal atoms into graphene**
12:35 – 12:55	Silvan Kretschmer	**Understanding defect production in 2D materials under ion irradiation from advanced first-principles calculations**

Program

Monday, 8 May 2023

13:00 – 14:30	*LUNCH*	

Chair: Matthias Batzill

14:30 – 15:15	Andrey Turchanin	**Influence of intrinsic and extrinsic defects on the electronic and photonic properties of TMD monolayers**
15:15 – 16:00	Alexandra Radenovic	**Nanofluidics-next frontiers with hBN**
16:00 – 16:20	Łukasz Gelczuk	**Native Point Defects in Transition Metal Dichalcogenides - Experimental Verification of Theoretical Prediction**
16:20 – 17:00	*COFFEE BREAK*	
17:00 – 19:15	**NETWORKING**	
19:30	*DINNER*	

Program

Tuesday, 9 May 2023

08:00	*BREAKFAST*	

Chair: Oleg Yazyev

09:00 – 09:45	Steven Louie	**Excitons and Photophysics of 2D Materials: Effects of Defects and Moiré Structures**
09:45 – 10:30	Wouter Jolie	**Correlated quasiparticles in MoS_2 mirror twin boundaries on graphene**
10:30 – 10:50	Christopher Leist	**Deep learning-supported in-situ HRTEM experiments on graphene**
10:50 – 11:30	*COFFEE BREAK*	

Chair: Wouter Jolie

11:30 – 12:15	Oleg Yazyev	**Graphene nanoribbon junctions as elementary components of nanoelectronic circuits**
12:15 – 12:35	Laura Susana	**Atomic scale mapping of the electric field and charge density in BN nanostructures by 4D-STEM**
12:35 – 12:55	Manuel Längle	**Creation of noble gas clusters in a graphene sandwich through low energy ion irradiation**
12:55 – 13:00	**Conference photo** *(in front of the lecture hall)*	
13:00 – 14:30	*LUNCH*	

Program

Tuesday, 9 May 2023

Chair: Richard Wilhelm

14:30 – 15:15	Lino Pereira	**Functionalization of 2D materials using ultralow energy ion implantation**
15:15 – 16:00	Alex Belianinov	**Low Energy Implantation with Focused Ion Beams**
16:00 – 16:20	Mahdi Ghorbani-Asl	**The role of defects and impurities in the formation of crystals between bi-layer graphene upon alkali metal atom intercalation**
16:20 – 17:00	*COFFEE BREAK*	

Chair: Arkady Krasheninnikov

17:00 – 17:45	**Poster flashes 1**
17:45 – 19:15	**Poster session 1**
19:30	*DINNER*

Program

Wednesday, 10 May 2023

08:00	*BREAKFAST*	

Chair: Nasim Alem

09:00 – 09:45	Kazutomo Suenaga	**Electron microscopy and spectroscopy of 2D hybrid materials**
09:45 – 10:30	Jani Kotakoski	**Electron irradiation-induced defects in 2D materials in vacuum and in low-pressure atmospheres**
10:30 – 10:50	Michael Kiarie Kinyanjui	**How do atomic-scale lattice defects modulate ordered electronic phases in 2D quantum materials?**
10:50 – 11:30	*COFFEE BREAK*	

Chair: Jani Kotakoski

11:30 – 12:15	Richard Wilhelm	**Extended defect production in 2D materials by the impact of individual slow highly charged ions**
12:15 – 12:35	Zahra Fekri	**Modification of charge transport in single-layer MoS2**
12:35 – 12:55	Piotr Żemojtel	**First-principles analysis of the point-defects influence on spectroscopic properties of CdSe nanoplatelets**
13:00 – 14:30	*LUNCH*	
14:30 – 18:30	***EXCURSION***	
19:00	***HERAEUS DINNER*** *(social event with cold & warm buffet with complimentary drinks)*	

Program

Thursday, 11 May 2023

08:00	*BREAKFAST*	

Chair: Alex Belianinov

09:00 – 09:45	Hannu-Pekka Komsa	**Simulating Raman spectra of defective 2D materials**
09:45 – 10:30	Marija Drndić	**Sculpting of 2D Materials: From Pores and Nanoporous Membranes**
10:30 – 10:50	Sadegh Ghaderzadeh	**Ab Initio Molecular Dynamics Simulations of Metal-Particles Landing on Pristine and Defective Two-Dimensional Materials in Sputter Deposition Experiments**
10:50 – 11:30	*COFFEE BREAK*	

Chair: Marija Drndić

11:30 – 12:15	Adam Gali	**Defect spins and qubits in hexagonal boron nitride from first principles theory guiding experiments**
12:15 – 12:35	Nasim Alem	**High-resolution S/TEM Imaging and Cathodoluminescence of 2D MoSe2/WSe2 Nanodot/Matrix In-plane Heterostructures**
12:35 – 12:55	Barbara Maria Mayer	**Point defects in monolayer h-BN created by low energy argon irradiation and characterized through scanning transmission electron microscopy**
13:00 – 14:30	*LUNCH*	

Program

Thursday, 11 May 2023

Chair: Bruno Schuler

14:30 – 15:15	Chih-Kang Shih	**Scanning tunneling spectroscopy of van der Waals bilayers - from moire superlattices to moire quasicrystals**
15:15 – 15:35	Alexander Markevich	**Oxygen-mediated defect formation and degradation in 2D MoS2 and MoTe2**
15:35 – 15:55	Francis Davies	**Interface Defect Engineering and Morphological Control of Lateral 2d Heterostructures**
16:00 – 16:20	Maja Groll	**Investigation of the atomic electric field distribution in pristine and defective 2D WSe2 by differential phase contrast STEM**
16:20 – 17:00	*COFFEE BREAK*	

Chair: Arkady Krasheninnikov

17:00 – 17:45	**Poster flashes 2**
17:45 – 19:15	**Poster session 2**
19:30	*DINNER*

Program

Friday, 12 May 2023

08:00	*BREAKFAST*	

Chair: Hannu-Pekka Komsa

09:00 – 09:45	Bruno Schuler	**Single dopants in transition metal dichalcogenides under the scanning probe microscope**
09:45 – 10:30	Sarah Haigh	**Surfaces and Interfaces in Transition Metal Dichalcogenides studied by Advanced Transmission Electron Microscopy**
10:30 – 10:50	Renu Rani	**Single photon emitters in hBN via ultra-low energy helium ion implantation**
10:50 – 11:30	*COFFEE BREAK*	

Chair: Thomas Michely

11:30 – 12:15	Vincent Meunier	**Quantum theory of sputtering rates in 2D materials by transmission electron microscopy**
12:15 – 12:35	Scientific organizers	**Closing remarks & poster awards**
12:35 – 13:30	*LUNCH*	

End of the seminar and departure

NO DINNER for participants leaving on Saturday or Sunday; however, a self-service breakfast will be provided on Saturday, on Sunday self-catering!