

I N V I T A T I O N

Department of Condensed Matter Physics

Is pleased to invite you to the lecture

Recombination processes and carrier transport in nitride heterostructures: Insights from atomistic and multi-scale simulations

by

Dr. Stefan SchulzSchool of Physics, University College Cork, Cork, T12 YN60, Ireland
Tyndall National Institute, University College Cork, T12 R5CP, Ireland

Email: stefan.schulz@tyndall.ie

Date: 27 November 2024**Time:** 11:00**Venue:** Lecture room F1, Building 6, Faculty of Science, Kotlářská 2, Brno

Semiconductor nanostructures utilizing indium gallium nitride, (In,Ga)N, alloys have attracted considerable research interest due to their potential for optoelectronic device applications [1] but also recently as sources for non-classical light emission [2]. However, and in comparison to other III-V semiconductor heterostructures, (In,Ga)N-based systems exhibit very different fundamental properties. This starts with the underlying crystal structure (wurtzite vs. zincblende), ranges over to the presence of very strong electrostatic built-in fields and ultimately the observation of significant carrier localization effects in (In,Ga)N alloys [3]. In this talk, the impact of (random) alloy fluctuations on charge carrier transport, radiative and non-radiative recombination processes in (In,Ga)N-based heterostructures will be discussed.

Initially we will focus our attention on the temperature and carrier density dependence of the radiative and non-radiative (Auger) recombination in (In,Ga)N quantum wells, using an atomistic tight-binding model [4, 5, 6]. Equipped with this knowledge, consequences for the thermal and current “droop” in (In,Ga)N-based light emitting diodes will be discussed [7]. In addition, we will present our approach to address the impact of random alloy fluctuations on the charge carrier transport in (In,Ga)N-based devices, employing a multi-scale simulation framework. Results for uni-polar and bi-polar transport in (In,Ga)N multi-quantum well systems will be presented [8, 9].

In a second step, the electronic and optical properties of ultrathin, quasi-two dimensional (In,Ga)N layers embedded in GaN will be discussed [10]. These systems should ideally circumvent the quantum confined Stark effect and thus the spatial separation of charge carriers, which limits the efficiency of the “conventional” (In,Ga)N quantum well systems mentioned above.

Finally, consequences of random alloy fluctuations for non-classical light emission, e.g. polarization entangled or twin photons, from (In,Ga)N quantum dots will be discussed [11]. Here, results from a fully atomistic many-body framework, combining tightbinding electronic structure theory and a configuration interaction scheme, will be presented.

Co-funded by
the European UnionMINISTRY OF EDUCATION,
YOUTH AND SPORTS

References

- [1] C. J. Humphreys, MRS Bulletin 33 (2008), 459.
- [2] H.-S. Yeo et al., Nano Lett. 20 (2020), 8461.
- [3] P. Dawson et al., J. Appl. Phys. 119 (2016), 181505.
- [4] J. M. McMahon et al., Appl. Phys. Lett. 116 (2020), 181104.
- [5] J. M. McMahon et al., Phys. Rev. B 105 (2020), 195307.
- [6] R. M. Barret et al., ACS Photonics 10 (2023), 2632.
- [7] M. Meneghini et al., J. Appl. Phys. 127 (2020), 211102.
- [8] M. O'Donovan et al., J. Appl. Phys. 127 (2021), 065702.
- [9] M. O'Donovan et al., Phys. Rev. Appl. 024052 (2024).
- [10] D. S. P. Tanner et al., Nanoscale 12 (2020), 20258.
- [11] S. K. Patra et al., Nano Lett. 20 (2020), 234.

Acknowledgments: This work was financially supported by Science Foundation Ireland (17/CDA/4789 and 12/RC/2276 P2). Furthermore, computing resources provided by Science Foundation Ireland (SFI) to the Tyndall National Institute and by the SFI and Higher Education Authority funded Irish Centre for High End Computing (ICHEC) are acknowledged.

This lecture was supported by the project QM4ST (Quantum materials for applications in sustainable technology), reg. no. CZ.02.01.01/00/22_008/0004572, cofunded by the ERDF from the Programme Johannes Amos Commenius, call Excellent Research.



Co-funded by
the European Union

