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CONTROLLED GENERATION OF LUMINESCENT CENTRES IN HEXAGONAL BORON NITRIDE BY IRRADIATION ENGINEERING

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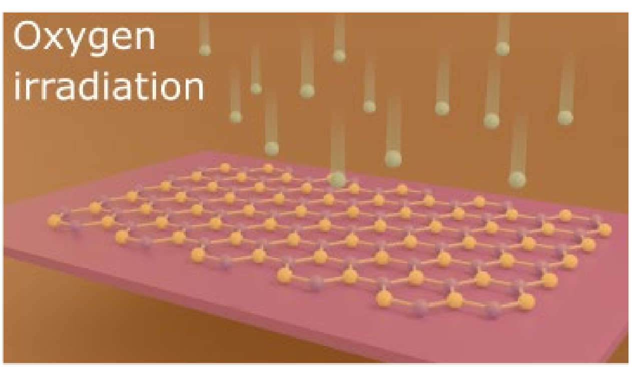
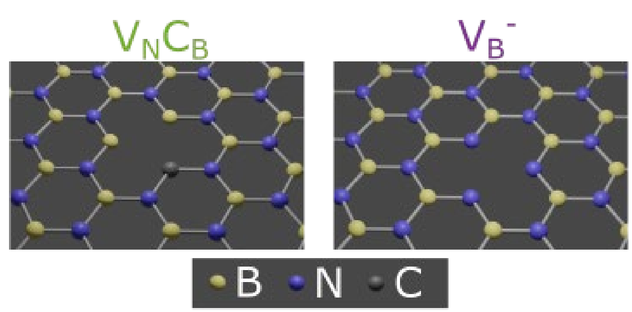
The discovery of room-temperature quantum emitters in the two-dimensional material hexagonal boron nitride (hbN) triggered a large number of research work since they have to potential to enable quantum applications without cryogenic systems [1]. In order to be utilized for applications it is crucial to find novel methods to generate these luminescent centres deterministically and on-demand as well as to identify their true microscopic nature. Here we present a novel method for generating luminescent centres inspired by irradiation engineering with oxygen atoms [2]. We explore systematically the influence of the kinetic energy as well as the irradiation fluence (defined as the number of oxygen atoms per area) on the density of luminescent centres. Both parameters modify the density while a significant, five-fold enhancement is observed with increasing fluence. Molecular dynamics simulations in combination with experimental findings clarify the generation process of these luminescent centres. We identify the most likely defects formed, namely V_NC_B and V_B^- as shown below. *Ab initio* calculations of these defects show excellent agreement with the experimental photoluminescence line shapes. The presented methodology, i.e. irradiation engineering compared with molecular dynamical and *ab initio* calculations, allows us to generate deterministically quantum emitters in hBN and to provide insights into their microscopic origin. The presented irradiation engineering is wafer-scalable and could be adapted to other irradiating atoms or ions as well as other gapped 2D materials.





[1] T. T. Tran *et al.* Quantum emission from hexagonal boron nitride monolayers, Nature Nanotechnology **11,** 37 (2016).
[2] M. Fischer *et al.* Controlled generation of luminescent centres in hexagonal boron nitride by irradiation engineering, Science Advances **7,** in press (2021).