

Excitons and magnons in 2D crystals with the XATU code

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Excitons play a central role in determining the optical properties of two-dimensional (2D) crystals such as hexagonal boron nitride or transition metal dichalcogenides. These properties range from simple light absorption to non-linear responses [1]. Methodologically, the Bethe-Salpeter equation (BSE) has become the corner stone for the computation of excitons. In my talk, I will present the **XATU** initiative [2], a toolbox with the implementation of such an equation with the aim to cover the whole range of computational complexity and accuracy, from simple effective models [2] to fully ab initio calculations [3] (see Fig. 1), along with the resulting linear and non-linear optical responses [4]. Also, I will present our efforts to compute magnons in magnetic 2D crystals from the very same BSE.

References

- [1] MA García-Blázquez, JJ Esteve-Paredes, AJ Uría-Álvarez, JJ Palacios, *Journal of Chemical Theory and Computation* 19 (2023) 9416-9434.
- [2] AJ Uría-Álvarez, JJ Esteve-Paredes, MA García-Blázquez, JJ Palacios, *Computer Physics Communications* 295 (2024) 109001.
- [3] MA García-Blázquez, JJ Palacios, *Physical Review Research* 7 (2025) 013156
- [4] JJ Esteve-Paredes, MA García-Blázquez, AJ Uría-Álvarez, ...*npj Computational Materials* 11 (2025) 13.

Figures

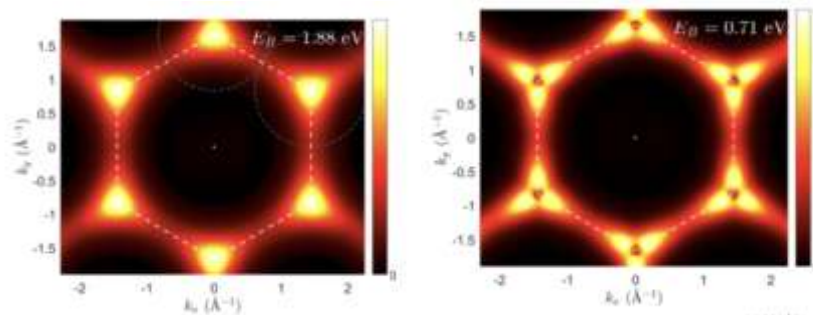


Figure 1: A bright (left) and a dark (right) exciton in hBN in reciprocal space.