

# EXCITONS IN VANDER WAALS MATERIALS: FROM MONOLAYER TO BULK HEXAGONAL BORON NITRIDE

J. Koskelo<sup>1</sup>, G. Fugallo<sup>2,3</sup>, M. Hakala<sup>1,4</sup>, M. Gatti<sup>2,3,5</sup>, F. Sottile<sup>2,3</sup>, and P. Cudazzo<sup>2,3</sup>

<sup>1</sup> Department of Physics, P.O.B. 64, FIN-00014 University of Helsinki, Finland

<sup>2</sup> Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA, Université Paris-Saclay, F-91128 Palaiseau, France

<sup>3</sup> European Theoretical Spectroscopy Facility (ETSF)

<sup>4</sup> Department of Chemistry, P.O.B. 16100, FIN-00076 Aalto, Finland

<sup>5</sup> Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette, France

email: jaakko.koskelo@helsinki.fi

Recently, the so-called van der Waals heterostructures have attracted interest due to the prospect of tailoring their properties by choosing suitable monolayer materials as building blocks. For this purpose, it is useful to understand the exciton properties of layered materials from the excitons of their constituent monolayers. Moreover, this kind of understanding may give access to deeper insight in the excitons of known layered materials. Motivated by these considerations, we have investigated the connection of monolayer and bulk excitons using hexagonal boron nitride (hBN) as an example system [1].

We performed first-principles calculations on momentum-dependent valence excitation spectra employing the Bethe-Salpeter equation (BSE), and interpret these results by a simplified model based on BSE. We discuss the exciton properties by considering the interplay of interlayer hopping and exchange electron-hole interaction. Furthermore, we discuss the relation of exciton and plasmon in hBN.

[1] J. Koskelo, G. Fugallo, M. Hakala, M. Gatti, F. Sottile, and P. Cudazzo, *Phys. Rev. B* **95**, 035125 (2017).