Excitonic effects in graphene-like C_3N

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Monolayer C_3N [1] is an emerging two-dimensional indirect band gap semiconductor with interesting mechanical, thermal and electronic properties. In this work we present a full description of C_3N electronic and dielectric properties, focusing on the so-called momentum-resolved exciton bandstructure (Fig.1). The study is performed using GW+BSE approach for zero and finite momentum transfer, as implemented in the Yambo code [2].
Excitation energies and oscillator strengths are computed in order to characterize bright and dark states. Activation of excitonic states is observed for finite transferred momentum. We find an indirect excitonic band gap of 0.8 eV, significantly lower than the direct optical gap of 1.96 eV. Excitonic binding energies ranging from 0.6 to 0.8 eV for the lowest excitonic states, are indicative of strongly bound excitons. Excitonic wavefunctions are discussed with respect to crystal symmetries.

References

[1] J. Mahmood et al., PNAS, 113, 7414 (2016)
[2] D Sangalli et al., J. Physics: Condens. Matter 31, 325902 (2019).

Figures

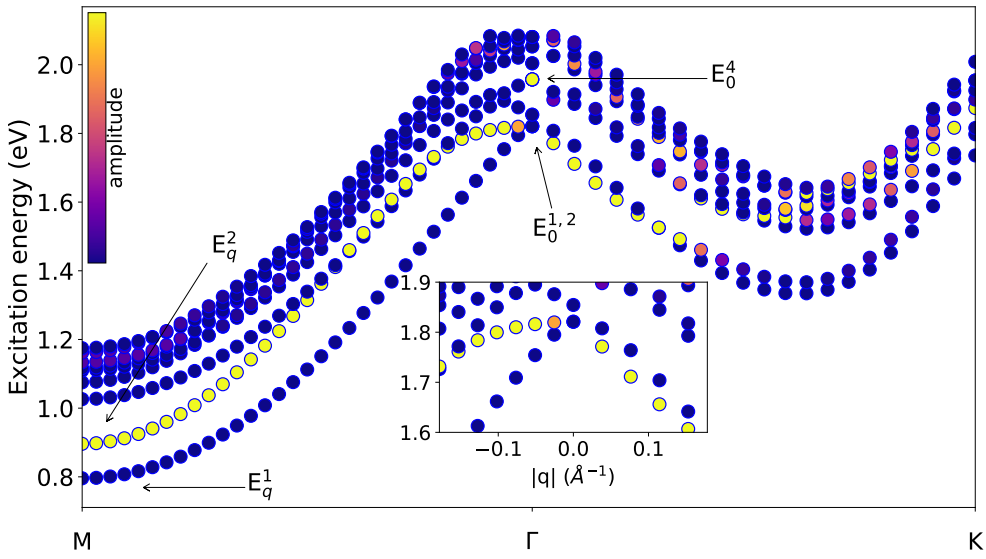

Figure 1: Momentum-resolved exciton bandstructure of C_3N for high-symmetry directions.