

Ab initio description of exciton dispersion

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Psi-k Conference
Donostia - San Sebastián
8 September 2015



Excitons

→ optical properties $\epsilon(\omega)$

↳ material description

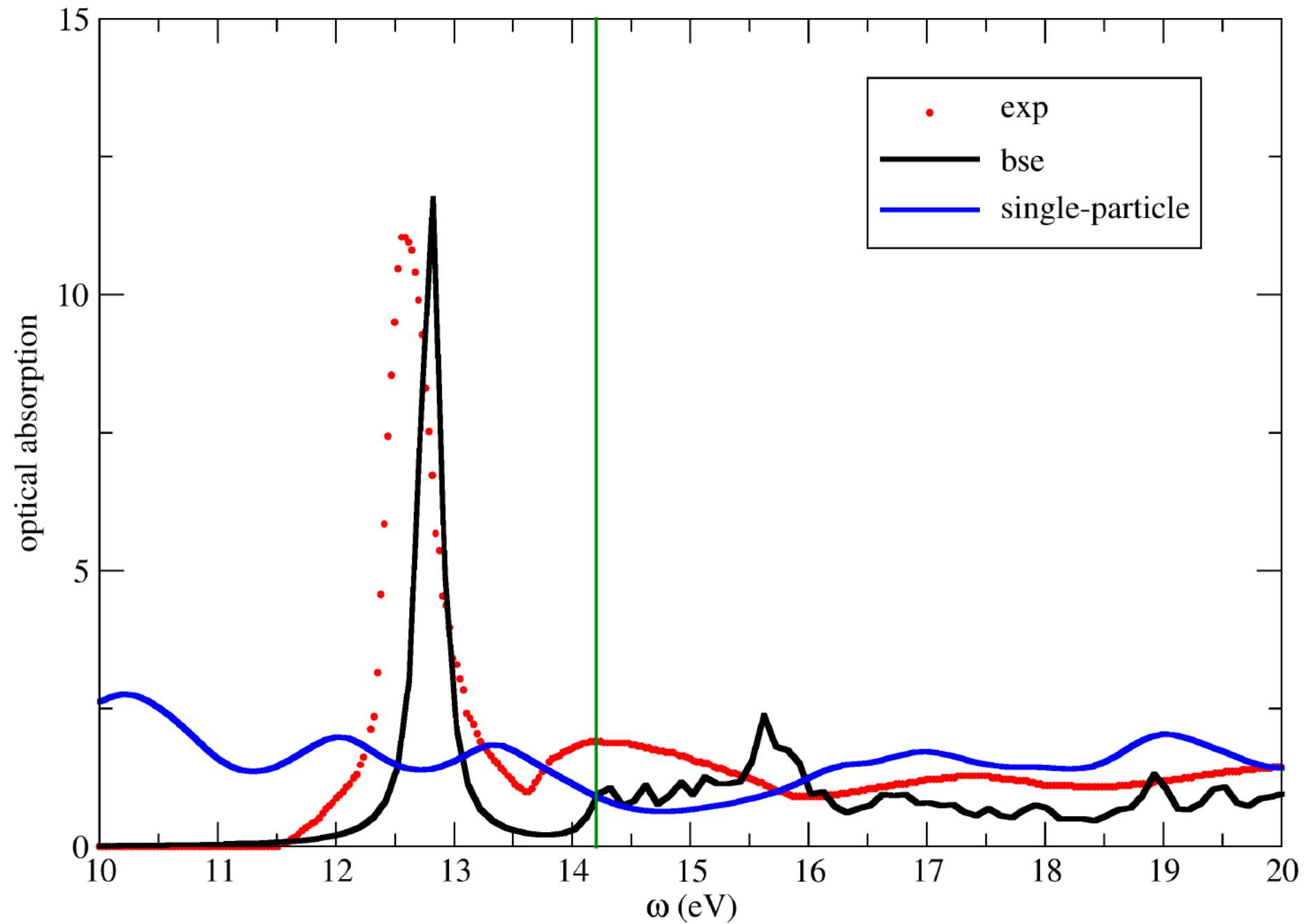
↳ applications (photovoltaics,
optoelectronics, phototherapy)

→ we need Bethe-Salpeter eq. (BSE)

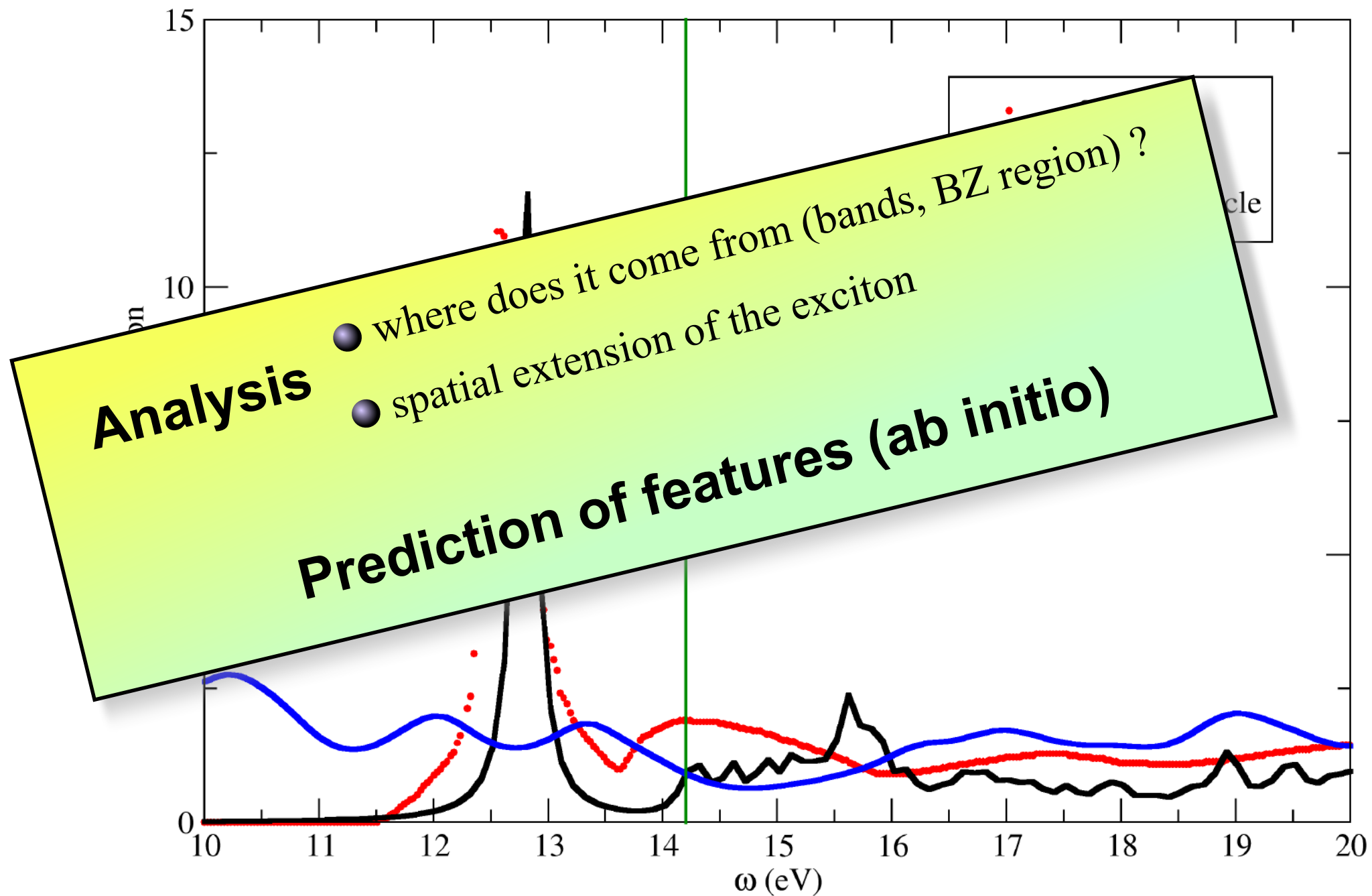
✗ cumbersome

✓ accurate
ab initio

Absorption spectrum of LiF

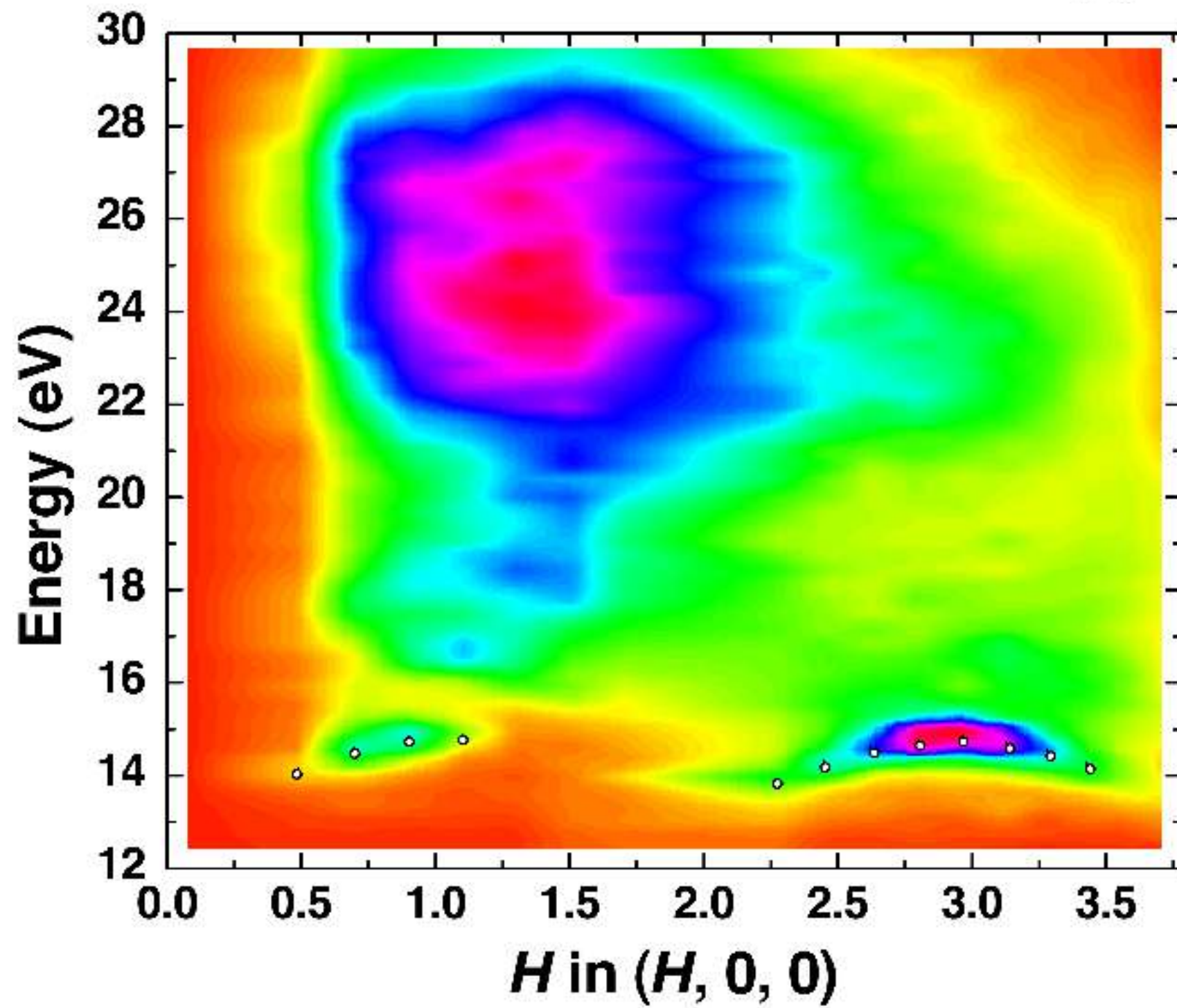


Absorption spectrum of LiF



Need to go beyond $\epsilon(\omega)$

- full screening $\epsilon(\mathbf{q},\omega)$ is required in many-body physics (photoemission spectroscopy, band-gap, etc.) beyond RPA
- EELS, IXS are able today to give a full mapping of $\epsilon(\mathbf{q},\omega)$ crucially requiring a theoretical description



Bethe-Salpeter Equation extension (q)

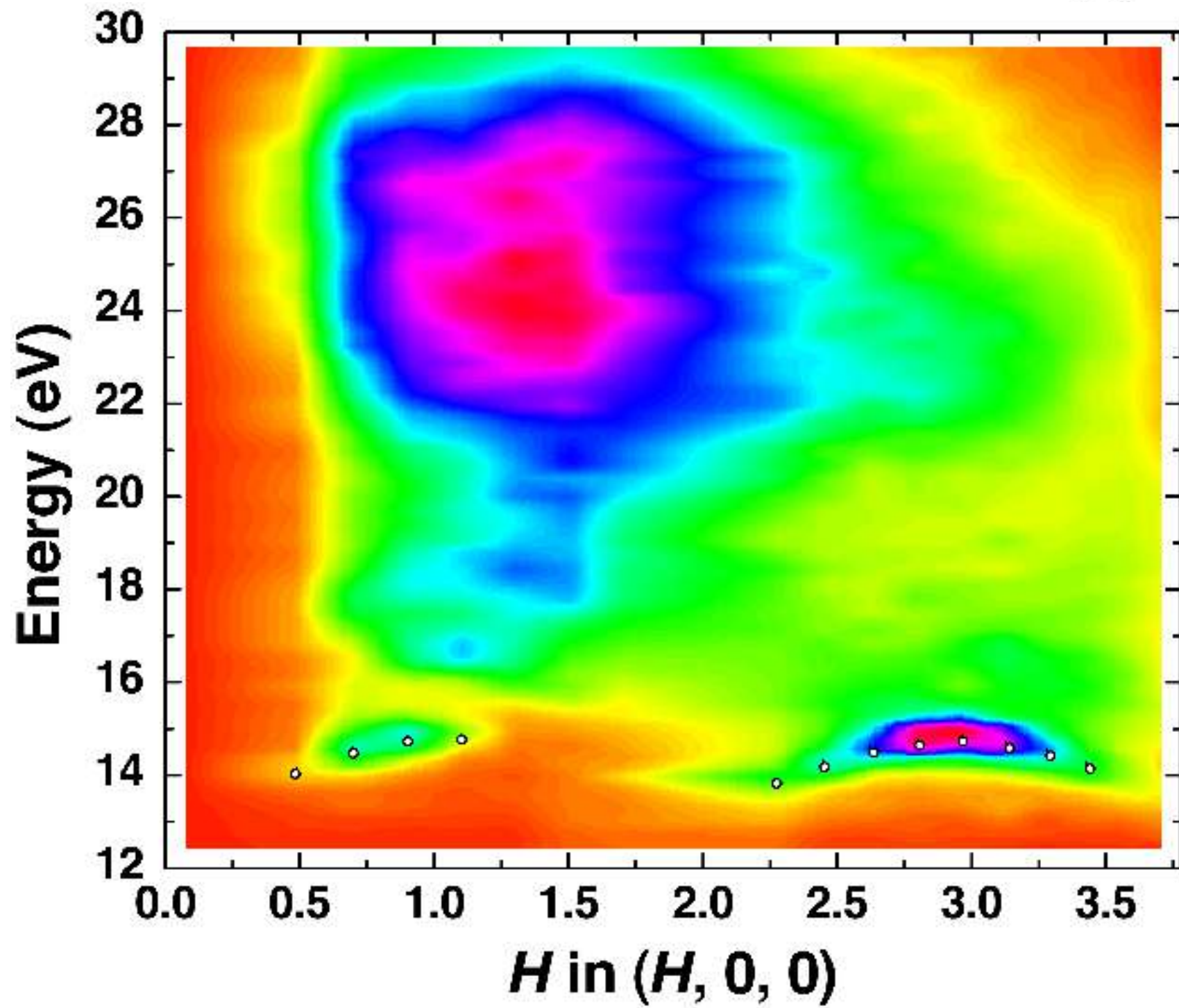


M. Gatti and F. Sottile PRB **88**, 85425 (2013)

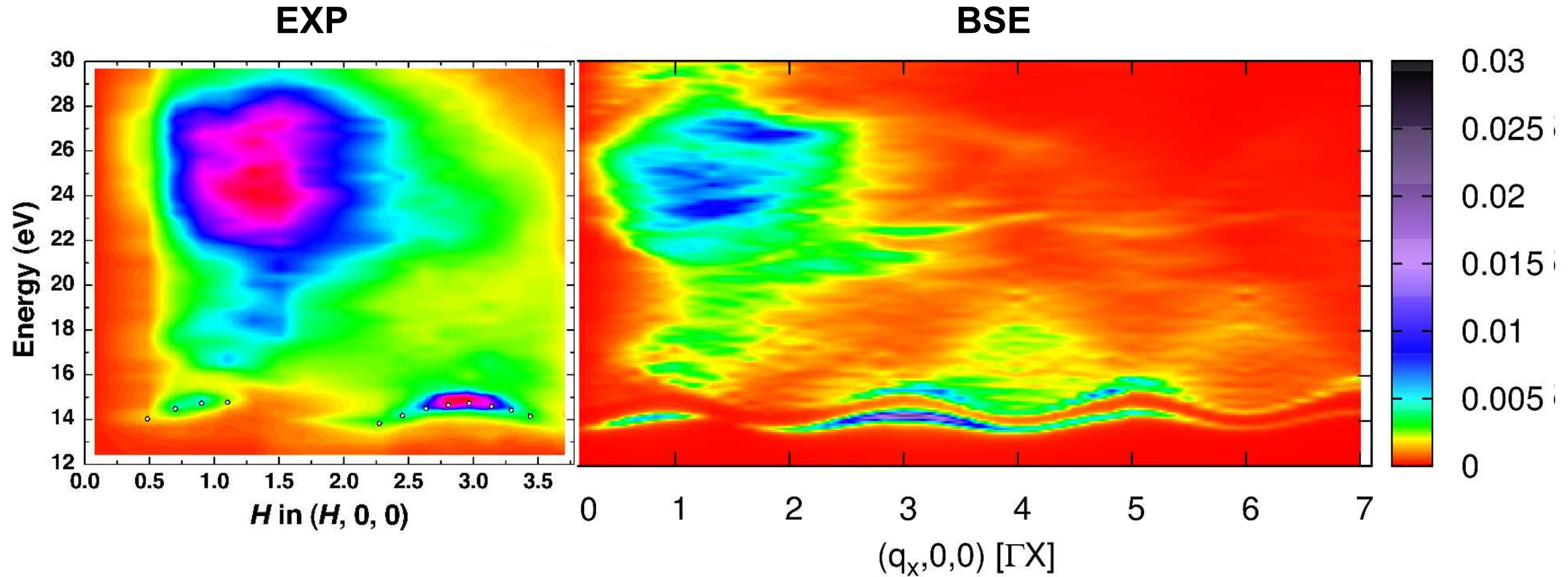


{ finite momentum transfer (beyond dipole)
quasi-particle wavefunctions
full coupling (beyond TDA)

EXC code www.bethe-salpeter.org/



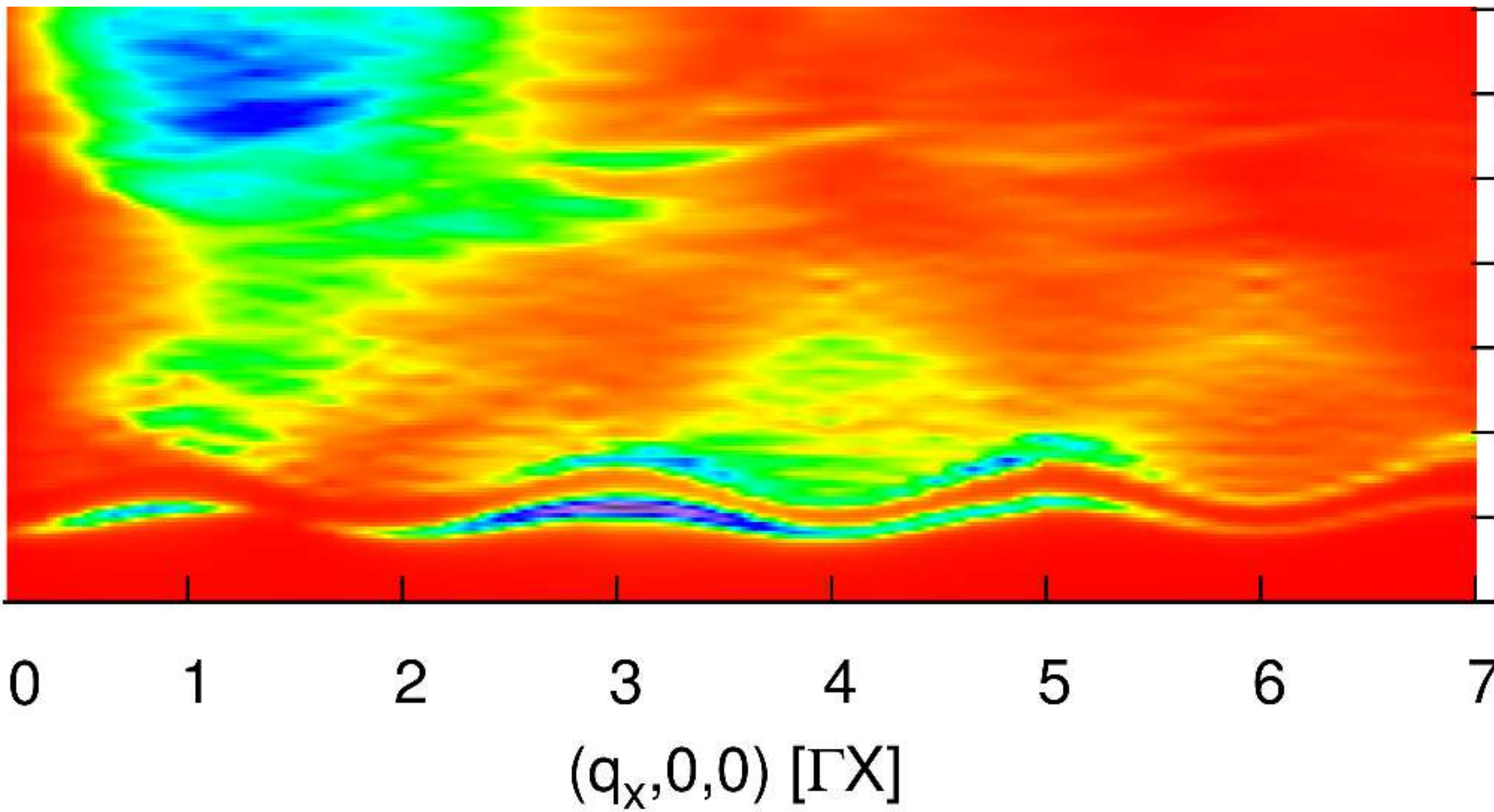
Dynamical Structure factor of LiF



P. Abbamonte et al. PNAS **105**, 12159 (2008);
Chi-Cheng Lee et al. PRL **111**, 157401 (2013)



M. Gatti and F. Sottile PRB **88**, 85425 (2013)

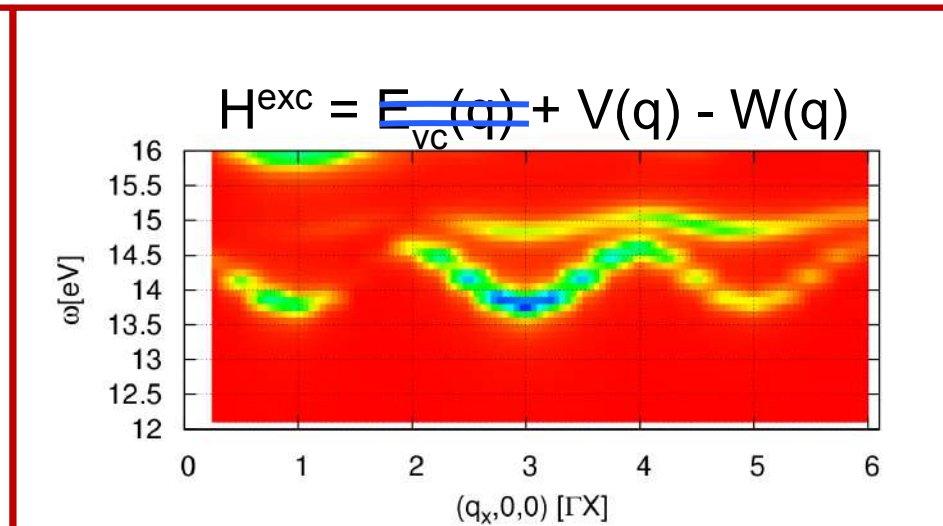
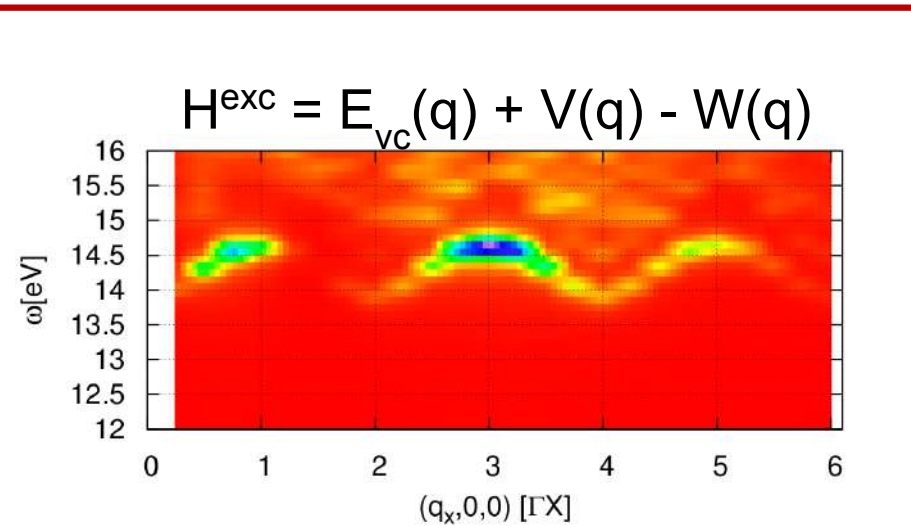


Analysis of the exciton dispersion

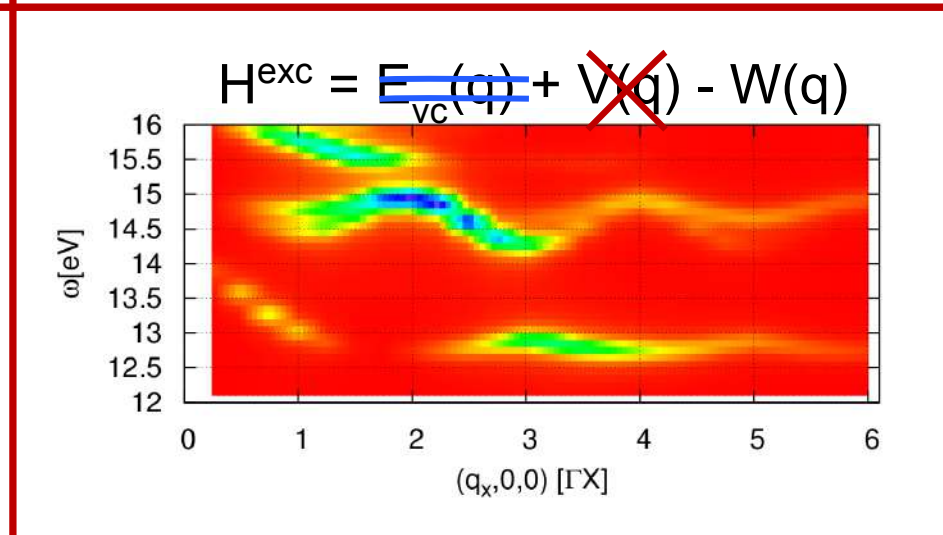
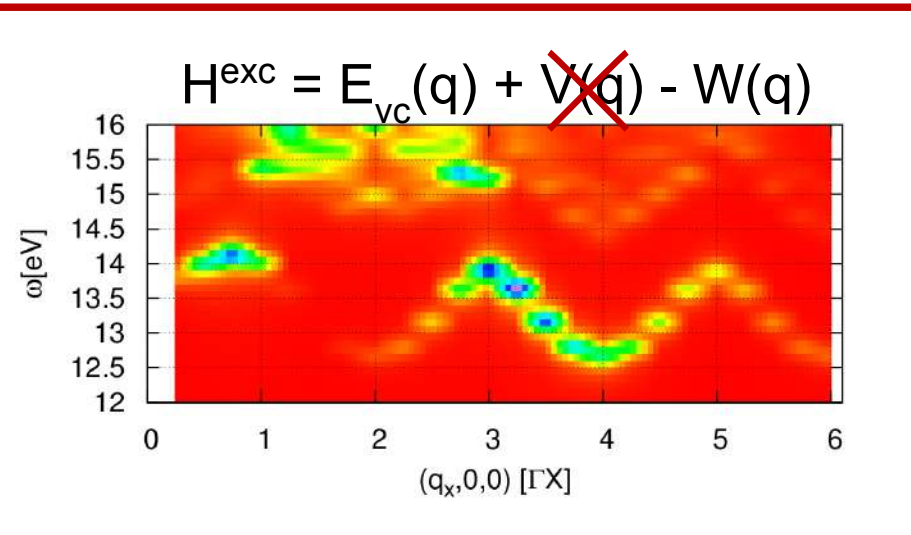
true bands

flat bands

singlet



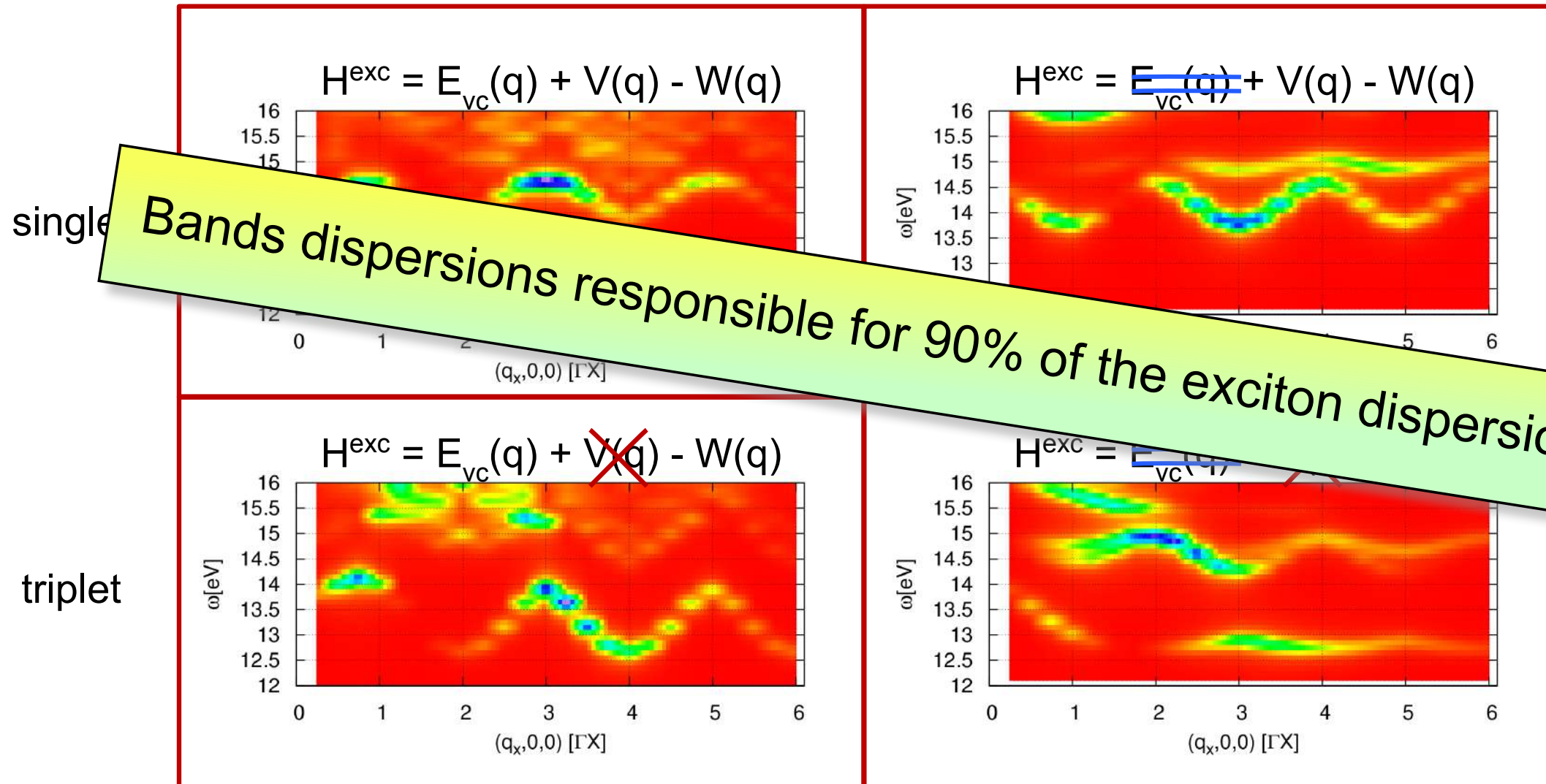
triplet



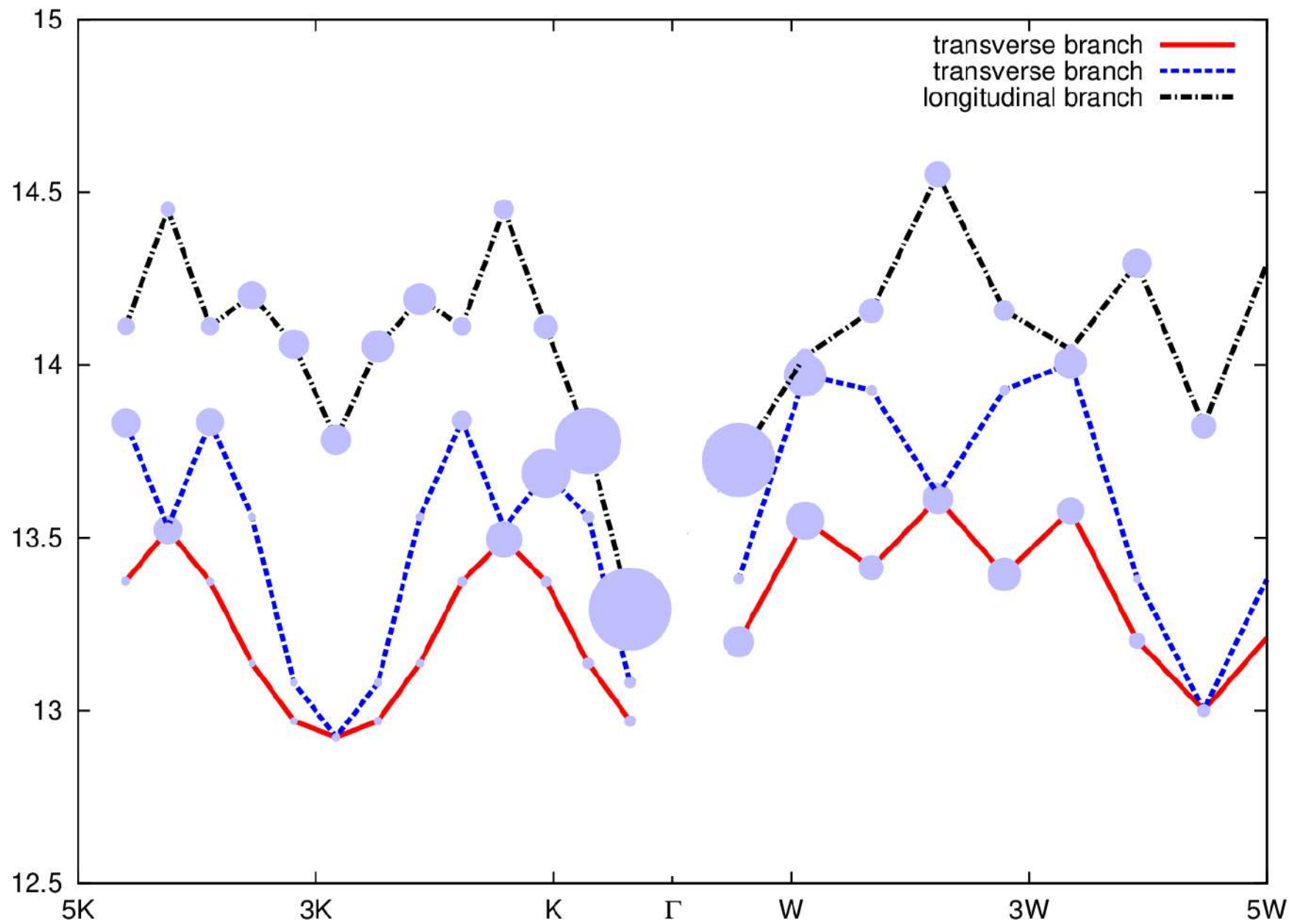
Analysis of the exciton dispersion

true bands

flat bands

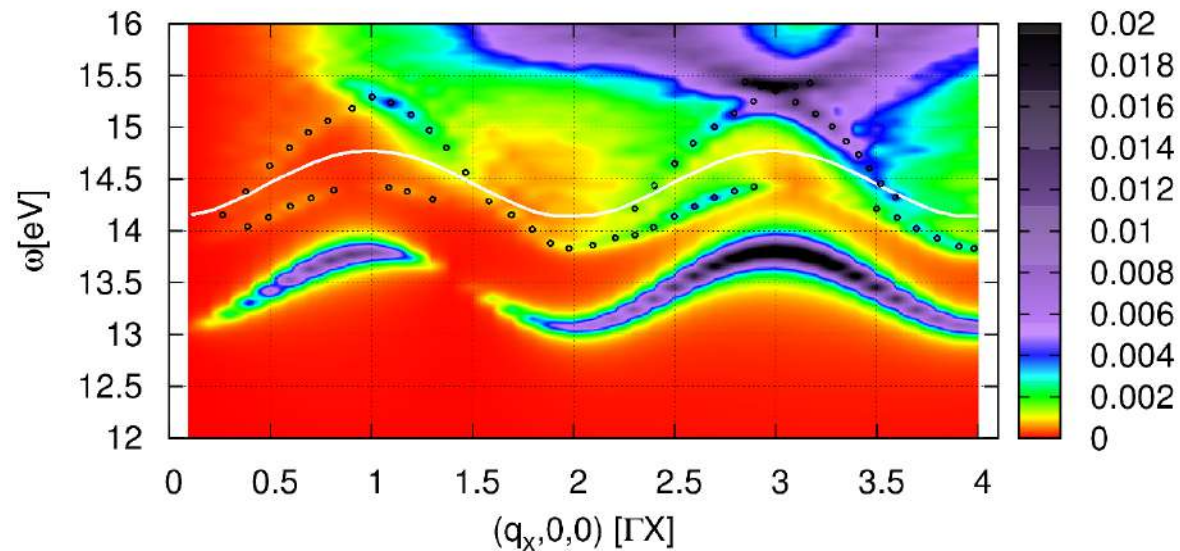


Excitonic bandstructure

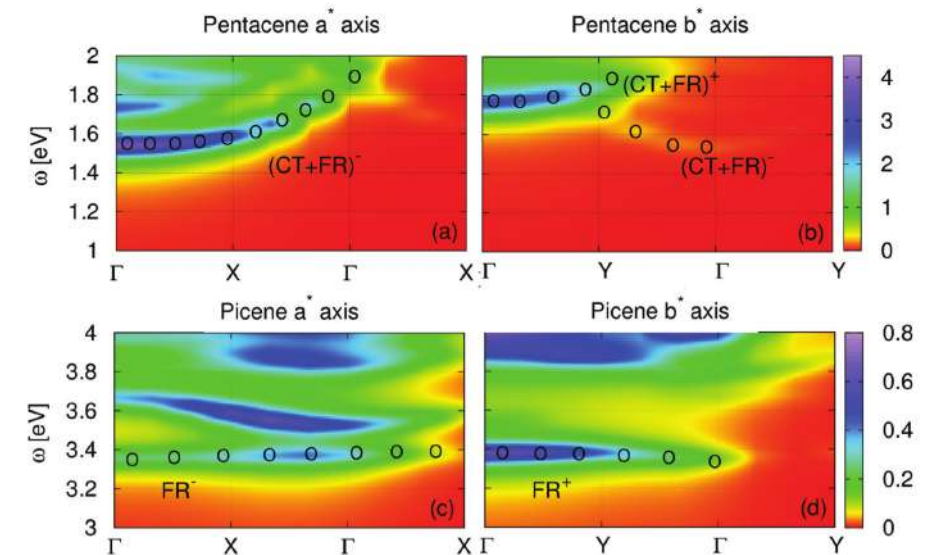


Exciton dispersion - not only LiF

predictions for Ar



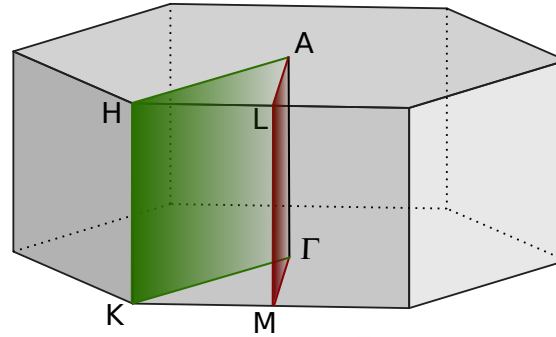
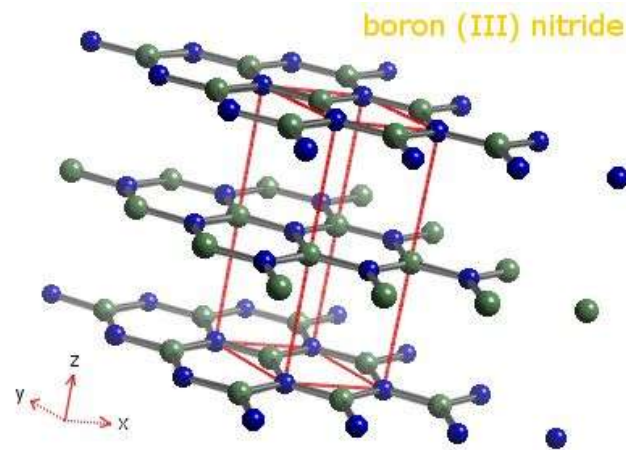
Molecular solids



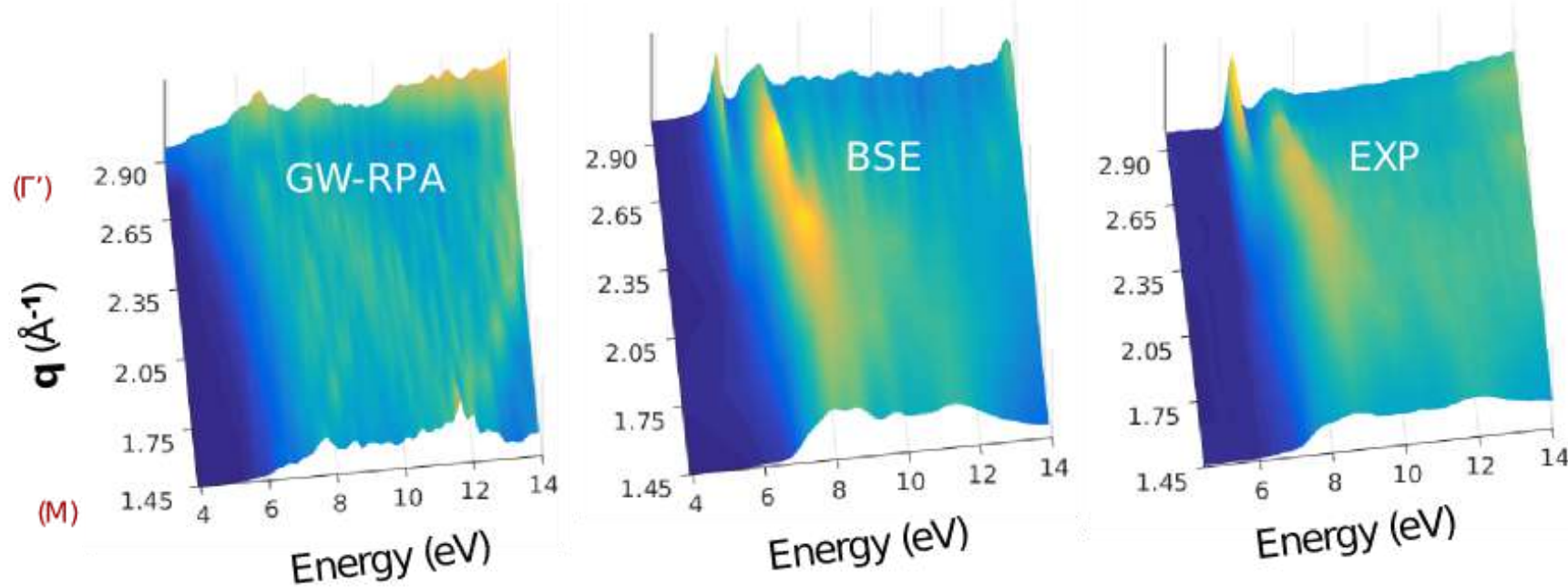
 M. Gatti and F. Sottile PRB **88**, 85425 (2013)

 P. Cudazzo, M. Gatti, A. Rubio and F. Sottile, PRB **88**, 195152 (2013)

Exciton dispersion - towards 2D



Giorgia Fugallo



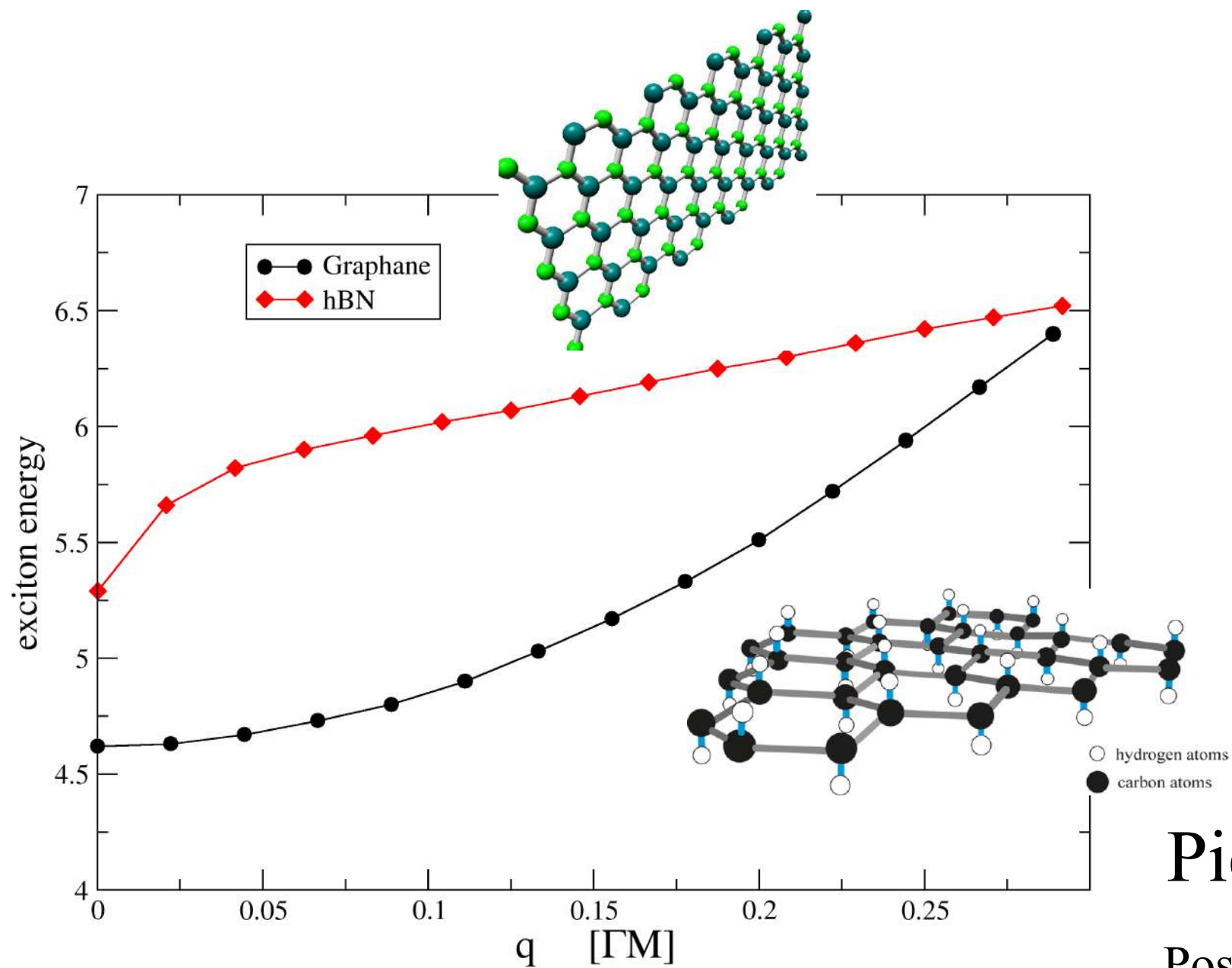
ID20 beamline 5/2015



G. Fugallo et al. arXiv <http://arxiv.org/abs/1508.01769> (2015)

Poster hBN, MoS₂

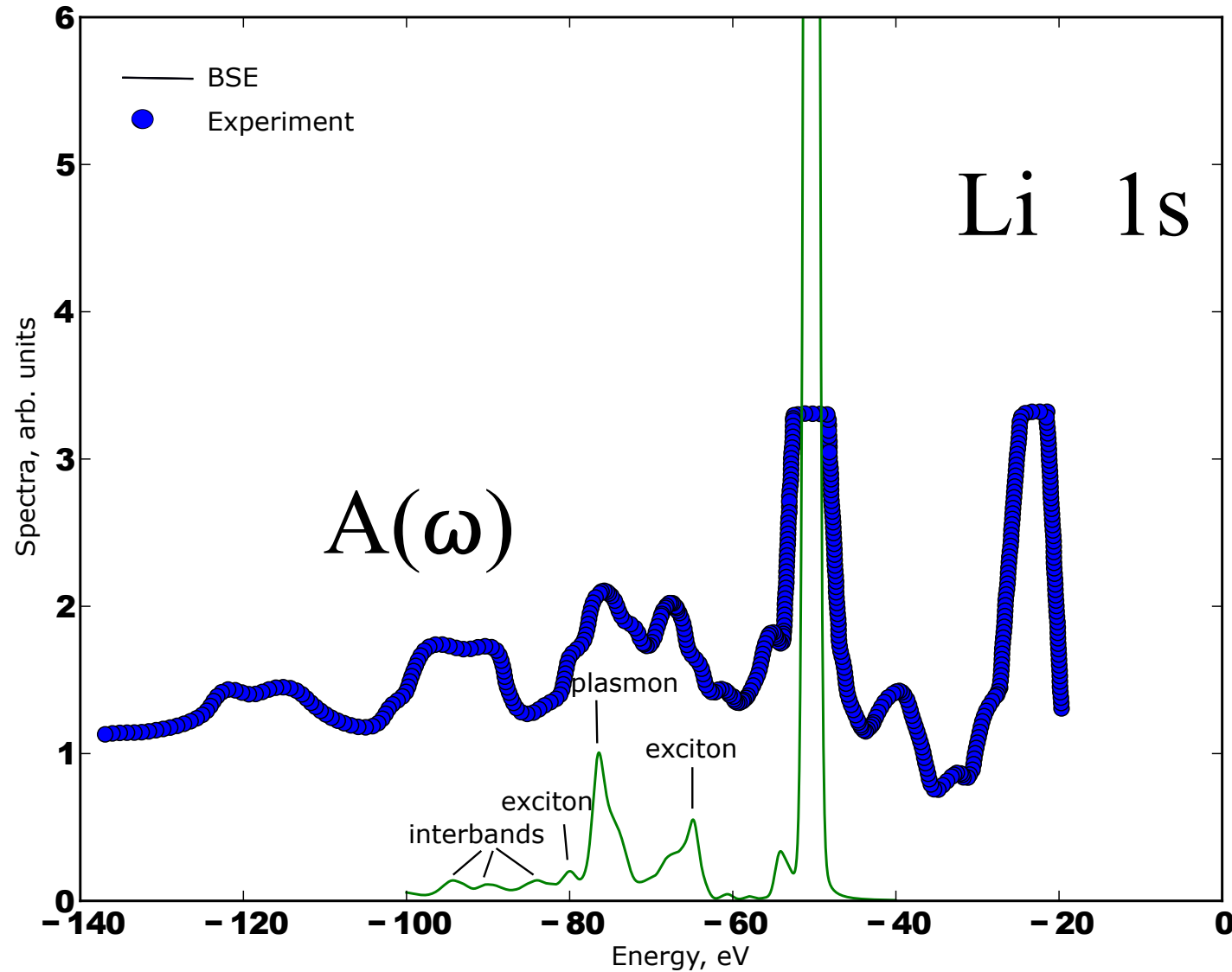
Exciton dispersion - 2D systems



Pierluigi Cudazzo

Poster 2D hBN, Graphane

Excitons Satellites in Photoemission



Igor Reshetnyak



Poster

M. Scrocco PRB 32, 1306 (1985).

Conclusions

- ➔ **Extension of BSE (q)**
- ➔ **Study several systems**
LiF, Ar, Molecular Solids
hBN, MoS₂, 2D systems
- ➔ **Excitonic effects in screening**
(exciton satellites in PES)
- ➔ **Other spectroscopies (CIXS, RIXS)**
Graphic visualization