

Exciton Dispersion of Insulators and Molecular Solids

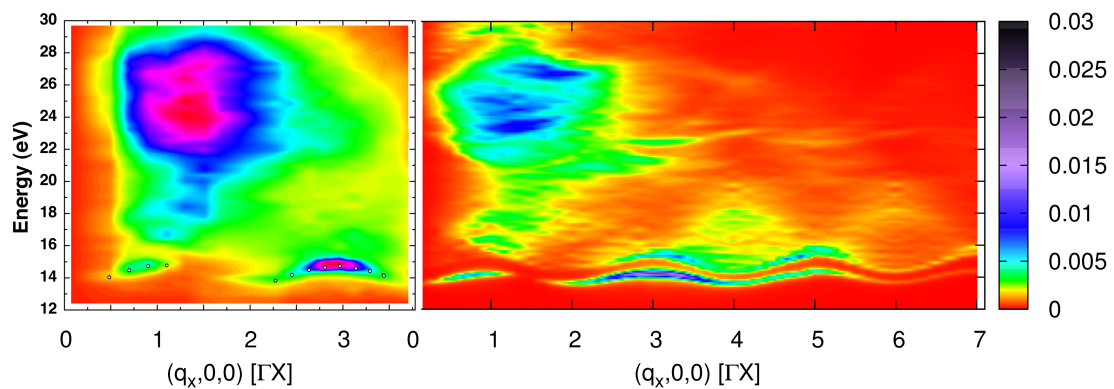
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We present ab initio calculation of plasmon and exciton dispersion of wide-gap insulators, like LiF or hBN, as well as molecular solids. With the help of the Bethe-Salpeter Equation (recently extended [1,2] to describe full coupling momentum excitonic effects) we calculate the momentum dispersion of the first low-lying excitons, both visible and dark. Their particular behaviour is analysed (with respect to momentum intensity and direction, coupling effect, real space distribution and interference effects) and the results are compared with recent inelastic X-ray scattering [3] and with electron energy loss spectroscopy [4,5].



Experimental (left panel) and theoretical (right) dynamical structure factor of LiF, as a function of momentum transfer and energy loss.

Références

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