

Abstract Submitted
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**Dynamical structure factor of LiF for all wave vector transfers:
New results and insights**¹ Q. KOU, M.C. TROPAREVSKY, A.G. EGUILUZ(1),
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ORNL(2), P. ZSCHACK, APS-ANL(3) — We report a theoretical-experimental
investigation of the dynamical structure factor of LiF. The calculations are done
within the TDLDA of time-dependent density functional theory; the measurements
correspond to non-resonant inelastic x-rays scattering (NIXS) cross sections, ob-
tained in absolute units. The TDLDA spectra contain one adjustable parameter: a
“scissors-operator” shift of the conduction bands. This parameter is determined in
view of the NIXS line shape for $q=6\text{\AA}^{-1}$ ($q//(111)$). The TDLDA spectra display
a non-trivial semi-quantitative agreement with the NIXS data, for all wave vectors
(directed along the three high-symmetry directions); indeed, the line shape changes
drastically from the coherent-response small- q regime, to the incoherent-response
large- q regime. The picture of the excitations which emerges offers an alternative
view relative to a seminal investigation involving an approximate solution of the
Bethe-Salpeter equation; W. A. Caliebe et al. Phys. Rev. Lett. 84, 3907 (2000).

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