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Dynamical structure factor of CaF_2: Striking coherent dynamical screening of "atomic" Ca-derived excitations O.D. RESTREPO, M.C. TROPAREVSKY, A.G. EGUILUZ, U. Tennessee and ORNL, B.C. LARSON, J.Z. TISCHLER, ORNL, P. ZSCHACK, Cornell, Y.Q. CAI, H. ISHII, P. CHOW, NSRRC, Taiwan, E.L. SHIRLEY, NIST, C.C. KAO, BNL — We report *ab initio* calculations of the dynamical structure factor of CaF_2,performed within time-dependent density functional theory, together with non-resonant inelastic x-ray scattering measurements. The "effective" dielectric function has also been determined. The excitations derived from the "atomic" Ca 3p–> 3d process display a striking wave vector dependence. Such dipole-allowed excitation would be expected to lie at about 27 eV. *However, for small q's the leading Ca 3p–> 3d feature lies at about 35 eV.* We demonstrate that this feature corresponds to a collective mode, whose physics embodies a remarkable manifestation of crystal local-field effects induced by charge localization and their interplay with the dynamical screening at the "natural" 3p–> 3d energy. For intermediate $q's$, the 27 eV excitation emerges and coexists with the collective mode —thus highlighting the physics of the "atomic" 3p–>3d excitation in the condensed matter environment, which is controlled by dynamical coherent screening. For large $q's$ the Ca-derived spectrum consists of the "single-particle" Ca 3p–>3d excitation, together with the dipole-forbidden Ca 3s–>3d excitation.

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