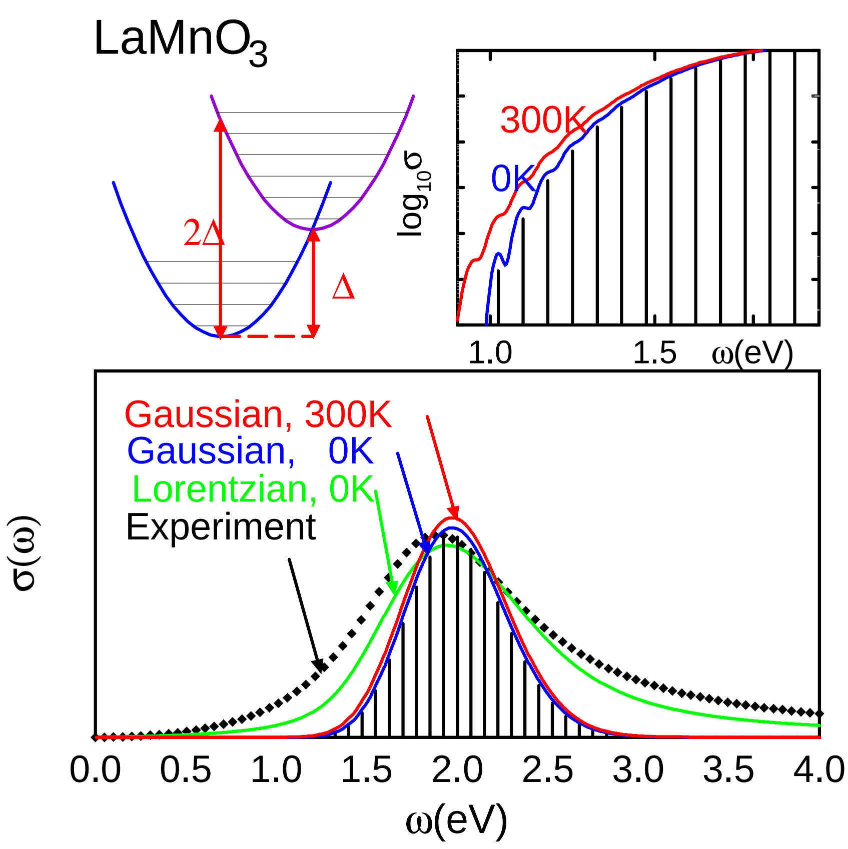
Self Trapped Exciton State

Phil Allen and Vasili Perebeinos have been working on the theory of small polarons in oxide materials. When an electron or a hole is inserted into an insulator, it often gets "self-trapped" by deforming the local lattice structure. This permits a localized bound state to form with a lower energy than simple insertion of an electron or hole into the conduction or valence band.

$LaMnO_3$ (Lanthanum manganite) is a fascinating material which has the potentially useful property known as "collossal magnetoresistance" when doped with holes (using partial substitution of Ca or Sr in place of La). When gently doped, $LaMnO_3$ remains insulating, presumably because potential current-carrying holes are self-trapped as small polarons. Allen and Perebeinos find that theory predicts self-trapping to occur also when an electronic excited state is created in the pure undoped material. Their predicted excitation spectrum is shown below, compared with optical experiments. In particular they suggest that transmission experiments on thin films should show weak absorption well below the main peak, with characteristic frequency and temperature dependence. This behavior, if confirmed experimentally, would serve as a fingerprint for self-trapping.



The spectrum is predicted to have the form of a "Franck-Condon series" of vibrational sidebands. In the absence of self-trapping, only the central band would appear. The experimental line-shape is broad, with only weak temperature dependence. The theory predicts that the low frequency wing of this broad line should show characteristic frequency-dependent and temperature dependent structure, illustrated in the log-scale version shown in the upper right.