Giant nonlinear electron-lattice interaction in cuprate superconductors, and origin of the pseudogap

DENNIS NEWNS, IBM T.J. Watson Research Center — The pseudogap is a key property of the cuprate superconductors, whose understanding should illuminate the pairing mechanism. Recent data support a close connection between the pseudogap and an oxygen-driven C4 symmetry breaking within the CuO$_2$ plane unit cell. Using $ab$ initio Molecular Dynamics, we show the existence of a strong nonlinear electron-oxygen vibrator coupling in two cuprates. In a mean field approach applied to this coupling, we derive a C4 splitting/pseudogap phase diagram in agreement with experiment - providing an explanation for the pseudogap phenomenon from first principles. The implications for superconductivity, Fermi surface arcing, and other properties are discussed.