

Abstract Submitted
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Possible enhancements of AFM spin-fluctuations in high- T_C cuprates THOMAS JARLBORG, DPMC, University of Geneva, CH-1211 Geneva 4, Switzerland — Ab-initio band calculations for high- T_C cuprates, together with modelling based of a free electron like band, show a strong interaction between anti-ferromagnetic (AFM) spin waves and periodic lattice distortions as for phonons, even though this type of spin-phonon coupling (SPC) is underestimated in calculations using the local density approximation. The SPC has a direct influence on the properties of the HTC cuprates and it can explain many observations. The strongest effects are seen for modulated waves in the CuO bond direction, and a band gap is formed near the X,Y points, but unusual band dispersion (like “waterfalls”) might also be induced below the Fermi energy (E_F) in the diagonal direction. The band results are used to propose different ways of increasing AFM spin-fluctuations locally, and to have a higher density-of-states (DOS) at E_F . Static potential modulations, via periodic distribution of dopants or lattice distortions, can be tuned to increase the DOS. This opens for possibilities to enhance coupling for spin fluctuations (λ_{sf}) and superconductivity. The exchange enhancement is in general increased near a surface, which suggests a tendency towards static spin configurations. The sensitivity of the band results to corrections of the local density potential are discussed.

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