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Theory of infinite-layer nickelate superconductors

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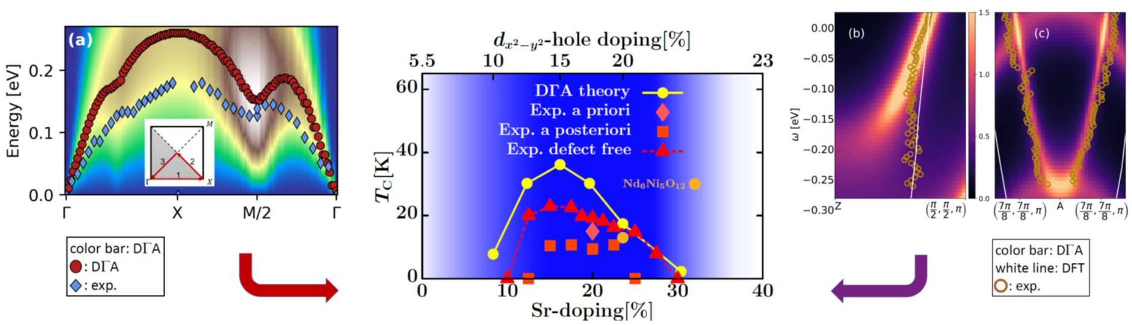
The discovery of superconductivity in infinite-layer nickelates [1] marked a new age of superconductivity: the nickel age. Using density functional theory, dynamical mean-field theory and dynamical vertex approximation (DΓA [2]), we successfully predicted the phase diagram T_c vs. Sr-doping of $Nd_{1-x}Sr_xNiO_2$ with -for an unconventional superconductor- unprecedented accuracy with "defect free" films synthesized only 3 years later [4]. Also, the normal state spin spectrum well agrees with resonant inelastic x-ray spectroscopy (RIXS) [5] and the one-particle spectrum with angular-resolved photoemission spectroscopy (ARPES) [6], which both enter into the calculation of T_c (as indicated by the arrows)

With this excellent agreement to later experiments, we can now with some confidence calculate the phase diagram of finite-layer nickelates [7] and predict that infinite-layer nickelates have a much higher T_c under 100GPa of pressure even without any chemical doping [8].



Center: Superconducting T_c vs. Sr-doping of $Nd_{1-x}Sr_xNiO_2$ comparing DΓA with experiments ("a priori" [1]; "defect free" [3]; $Nd_6Ni_5O_{12}$ [9]). **Left:** DΓA vs. RIXS [10]. **Right:** DΓA vs. ARPES [11].

References:

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