Continuing search for the origin of HTSC: DFT studies of selected copper oxide proxy structures reviewed and paths forward suggested

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In this presentation, we review our past attempts to uncover the pairing mechanism underlying high temperature superconductivity in copper oxide compounds and suggest possible paths forward.1, 2 One such path would be to derive and generalize pairing coupling functions to apply to DFT + U computed eigenstates in order to estimate Cooper pair coupling strengths arising from a combination of both lattice and spin excitations. Interestingly, such interactions were found in transition metal alums some 78 years ago as manifested in linking their respective Debye and Curie temperatures.3  We suggest repeating such experiments today on the copper oxide compounds as a function of hole/electron concentration, along with a possible computational strategy to pursue in the interpretation of the results4 to finally resolve the fundamental origin of high temperature superconductivity.

References:
1. Paul Grant, <http://meetings.aps.org/link/BAPS.2016.MAR.R25.8>
2. P.M. Grant, Journal of Physics: Conference Series 129 (2008) 012042 doi:10.1088/1742-6596/129/1/012042
3. C. Starr, Phys. Rev. 60, 241 (1941)
4. Paul Grant, <https://meetings.aps.org/Meeting/FWS17/Session/B2.10>