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The role of doping, pressure and composition on the creation of holes in high T_c cuprates CLAUDIA AMBROSCH-DRAXL, University Graz, TIMO THONHAUSER, Rutgers University , EUGENE YA. SHERMAN, University Toronto — We present a series of first-principles calculations for Hg based high T_c cuprates investigating the effect of pressure, doping, and composition on the formation of charge carriers. In particular, the total and site-projected hole concentration in the CuO_2 planes and the density of states are studied in detail. We also discuss effects of inhomogeneity introduced by doping and the limitations on creating holes by either doping, pressure, or the number of CuO_2 layers per unit cell. From an analysis and comparison of our results to available experimental data on the pressure dependence of T_c, we conclude that the effective coupling constant to the boson mediating the Cooper pairing is of the order of 1 ruling out the weak coupling approaches.

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