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Tuning the charge-transfer energy in hole-doped cuprates CHUCK-HOU YEE, Kavli Institute of Theoretical Physics, UCSB, GABRIEL KOTLIAR, Dept. of Physics & Astronomy, Rutgers University — Chemical substitution, combined with strain, allows the charge-transfer energy in hole-doped cuprates to be broadly tuned. We theoretically characterize the structural and electronic properties of the family of compounds $R_2CuO_2S_2$, constructed by sulfur replacement of the apical oxygens and rare earth substitutions in the parent cuprate La_2CuO_4. Additionally, the enthalpies of formation for possible synthesis pathways are determined.

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