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Rational design of novel thallium halide high T_c superconductors from first-principles ZHIPING YIN, GABRIEL KOTLIAR, Department of Physics, Rutgers University — Searching for new high-temperature superconductors remains one of the most active research areas in condensed matter physics and material physics. In this talk I will show how we designed, from first principles calculations, a novel family of thallium halide-based compounds as candidates for new high-temperature superconductors. This family together with the celebrated (Ba,K)BiO_3 and electron-doped HfNCl families are the "other high-temperature superconductors," whose superconductivity is mediated by the recently proposed mechanism of non-local correlation-enhanced strong electron-phonon coupling (arXiv:1110.5751). Two prototype compounds namely $CsTlF_3$ and $CsTlCl_3$ are studied with various hole doping levels and volumes. The critical superconducting temperature T_c are predicted to be about 30 K and 20 K with optimal hole doping and volume, respectively. Our procedure of designing this class of superconductors is quite general and can be used to search for other "other high temperature superconductors."

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