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Guided design of copper oxysulfide superconductors CHUCK-HOU YEE, TURAN BIROL, GABRIEL KOTLIAR, Rutgers University — Using the framework of chemical intuition introduced by Antipov, *et. al.*, in his synthesis of the Hg-based high-temperature superconductors, supplemented with modern first-principles electronic structure tools, materials databases, and evolutionary algorithms capable of exploring large configurational spaces, we design a novel family of copper oxysulfides. We explore the predictions of theories based on charge-transfer energies, orbital distillation and uniaxial strain on the superconducting transition temperatures of these oxysulfides.

Chuck-Hou Yee
Rutgers University

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