Material Specific Characterization Dataset (MSCD): A Novel Computational System for Searching for High-Tc Superconductors
MICHAEL SCHAFFER, O'PAUL ISIKAKU-IRONKWE[1], RTS Technologies, San Diego, CA 92126 — The search for novel high-Tc superconductors, HTSCs, involves billions of potential permutations and combinations in over 80 potential elements with thousands of structures. The need arises therefore for a quick-search system with predictive power. Using correlations of superconductivity with electronegativity, valence electrons, atomic number, formula weight, number of atoms and number of elements in the stoichiometry of superconductors, we have developed a simple predictive computational system called MSCD: Material Specific Characterization Dataset. MSCD of a superconductor defines and describes its stoichiometric structure in terms of averages of electronegativity, valence electrons, atomic number, formula weight, atoms-to-element ratio, ionic radii, first ionization energy and other associated ratios. We found that when the valence electrons and atomic numbers are the same, the materials have close Tcs. Also when the electronegativity and valence electrons are the same, they share the same crystal structure. Conversely, by tuning a material's stoichiometry to correspond to a known superconductor's MSCD, the material will become superconducting with close enough Tc. We give many examples of MSCD of superconductors and demonstrate the quick-search predictive power of MSCD in the search for novel HTSCs.

[1]The Center for Superconductivity Technologies (TCST), Michael Okpara University of Agriculture, Umudike, Abia State, Nigeria

Michael Schaffer
RTS Technologies, San Diego, CA 92126