Designing Superconductors with Periodic Table-based Maps and Material Databases

O. PAUL ISIKAKU-IRONKWE, The Center for Superconductivity Technologies, Abuja FCT, ALEX ANIMALU, Department of Physics and Astronomy, University of Nigeria, Nsukka — One of the grand challenges of superconductivity science is achieving a paradigm shift from discovery by serendipity to discovery by design. Empirical and heuristic rules have been a useful bridge in this desired direction. Many early superconductors were discovered by this method and by serendipity. DFT-based ab initio methods have often ignored empirical and experimental data. Here we propose that by using Periodic Table-based maps such as electronegativity spectrum maps, valence electron spectrum maps and atomic number spectrum maps for binary systems, $A_xB_y$, combined with data-mining of experimental material databases we can “reverse-engineer” many known superconductors. We demonstrate the power of this technique by predicting new and novel superconductors without recourse to DFT calculations.

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