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Materials Cartography: Representing and Mining Material Space Using Structural and Electronic Fingerprints COREY OSES, Duke Univ, OLEXANDR ISAYEV, DENIS FOURCHES, EUGENE MURATOV, UNC Chapel Hill, KEVIN RASCH, Duke Univ, ALEXANDER TROPSHA, UNC Chapel Hill, STEFANO CURTAROLO, Duke Univ, CENTER FOR MATERIALS GENOMICS, DUKE UNIVERSITY COLLABORATION, LABORATORY FOR MOLECULAR MODELING, UNC CHAPEL HILL COLLABORATION — As the proliferation of high-throughput approaches in materials science is increasing the wealth of data in the field, the gap between accumulated-information and derived-knowledge widens. We address the issue of scientific discovery in materials databases by introducing novel analytical approaches based on structural and electronic materials fingerprints. The framework is employed to (i) query large databases of materials using similarity concepts, (ii) map the connectivity of the materials space (i.e., as a materials cartogram) for rapidly identifying regions with unique organizations/properties, and (iii) develop predictive Quantitative Materials Structure-Property Relationships (QMSPR) models for guiding materials design. In this study, we test these fingerprints by seeking target material properties. As a quantitative example, we model the critical temperatures of known superconductors. Our novel materials fingerprinting and materials cartography approaches contribute to the emerging field of materials informatics by enabling effective computational tools to analyze, visualize, model, and design new materials.

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