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From Database to Materials SEYEDAYAT GHAZISAEED, BORIS KIEFER, New Mexico State University — Designing new materials with specific features is one of the main scientific and technological challenges, at present. Large experimental and computational efforts are devoted to reach this goal. Still, these efforts are largely based on trial and error strategies and the question arises how to guide and how to accelerate this design process. An approach that addresses both questions is based on the realization that large databases of material structures have been compiled since the advent of diffraction in the early 20^{th} century. In particular, the detailed analysis of these databases gives access to local structure and geometrical distortions. These distortions in turn, are at least partly responsible for magnetic and electronic properties of transition metal bearing compound. We will present results of our effort to develop and employ database search strategies that extend the ability of available crystal structure search engines. We will also discuss sample search results and how they may guide and accelerate material design.

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