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An Extensive Database of Electronic Structure Calculations between Transition Metals[1] SHEREEF SAYED, DIMITRIOS PAPACONSTANTOPOULOS, George Mason Univ — Density Functional Theory and its derived application methods, such as the Augmented Plane Wave (APW) method, have shown great success in predicting the fundamental properties of materials. In this work, we apply the APW method to explore the properties of diatomic pairs of transition metals in the CsCl structure, for all possible combinations. A total of 435 compounds have been studied. The predicted Density of States, and Band Structures are presented, along with predicted electron-phonon coupling and Stoner Criterion, in order to identify potential new superconducting or ferromagnetic materials. This work is performed to demonstrate the concept of high-throughput calculations at the crossing-point of Big Data and materials science.

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