MATCOR, a Program for the Cross-Validation of Material Properties Between Databases. JORGE MARQUEZ CHAVEZ, BORIS KIEFER, New Mexico State University — Many technological materials are currently improved using data analytics and Machine Learning methods. In this effort it is clear that the fidelity of the input data can affect the reliability of the model predictions. In our contribution we focus on the input data and their consistency between materials databases. We developed MATCOR, an open-source software to facilitate the initial data verification. MATCOR verifies material properties between AFLOW and Materials Project through materials chemistry and crystallography, as well as computational parameters. The capabilities of MATCOR are demonstrated for several examples. Density shows the highest correlation among the tested properties, 98% of the materials agree to within 2.6%. Bulk- and shear-moduli showed deviations of less than 10% for 79.4% and 65.1% of the materials, respectively. The classification in materials as non-magnetic/paramagnetic and metallic/gapped are consistent among the two databases for 91% and 73% of the materials, respectively. These examples show that MATCOR can be used to accelerate data curation and outlier identification, crucial prerequisites for model building and materials discovery.

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