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Strategies to Accelerate Materials Design SEYEDAYAT GHAZISAEED, BORIS KIEFER, New Mexico State University — The 21st century faces many technological and scientific challenges, and the ability to master these challenges will rely heavily on our ability to design and discover suitable sets of materials. Previous research shows that many electronic, magnetic and optical properties depend strongly on chemistry and the detailed arrangement of the coordinating ligands. In the effort to understand these correlations for d-elements and f-elements, crystal field theory has proven to be particularly useful. The crystal geometry can be determined experimentally for example through x-ray diffraction and the results have been collected and catalogued in databases. In this presentation, we will describe and discuss our efforts to correlate crystal structure databases with crystal field theory, other databases, and first-principle calculations. The goal is to accelerate the identification of sets of promising crystal structures and chemistries to address materials science and engineering challenges in the current century. As an example of the workflow, we consider CrO_2, and how the coordination environment effects electronic and magnetic properties beyond CrO_2 in the rutile structure which is known to be half-metallic.

Seyedayat Ghazisaeed
New Mexico State University

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