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Three parameter crystal-structure prediction for sp-d valent compounds

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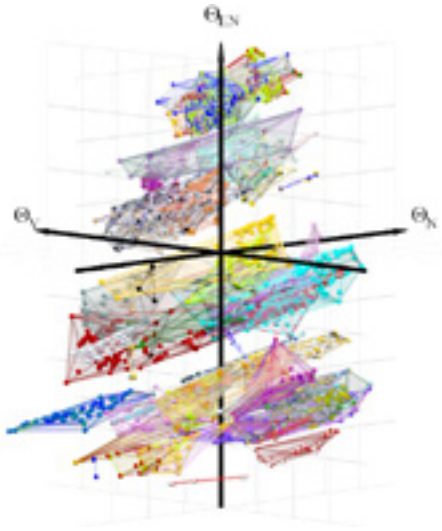
The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges in materials design. We use a cluster analysis of experimentally observed crystal structures and derive structure maps that are systematically optimized to reach high predictive power. In particular, we present a three-dimensional structure map for compounds that contain sp-block elements and transition metals in arbitrary composition. The structure map predicts the correct crystal structure with a probability of 86% and has a confidence of 98% that the correct crystal structure is among three predicted crystal structures. The three parameters that span the structure map are physically intuitive functions of the number of valence electrons, the atomic volume and the electronegativity of the constituent elements. We test the structure map against standard density-functional theory calculations for 1:1 sp-d-valent compounds and demonstrate that our three-parameter model has comparable predictive power. We show that the identified parameters are valid for off-stoichiometric compounds and they separate binary and ternary crystal-structure prototypes.



Figue-1: Three-parameter structure map for sp-d valent compounds. The colored polyhedrons correspond to different crystal-structures. The three descriptors are physically intuitive functions of electron count (N), atomic size (V) and electro-negativity (EN).

Biography

Thomas Hammerschmidt has his expertise and passion on the reliable and robust prediction of structural stability and phase stability of technologically relevant materials. In order to make direct contact to experiments, he includes finite temperature, complex microstructures and multi-component chemistry. His focus is particularly the development, implementation and application of analytic bond-order potentials for large scale atomistic simulations.

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