FAIR Semantic-Driven Analysis of Defect Properties in Metals

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Atomistic defect properties, such as stacking fault energies, are inherently challenging to simulate and calculate due to their complexity. A variety of methodologies, including gamma surface analysis, axial next-nearest neighbor Ising (ANNNI) models, and tilted cell approaches, are commonly employed to simulate these properties. The selection of computational parameters, such as the chosen force field and system configurations, determines the results of these computations. Consequently, the results are often highly sensitive to methodological choices, raising an important question: how can we ensure meaningful comparison as well as reproducibility of findings derived from different approaches?

Formalized frameworks to represent knowledge, such as ontologies, address this challenge by standardizing the representation of both data and methodologies and their relationships. Such a framework not only facilitate comparability across studies but also enhance reusability, enabling the systematic application of knowledge in subsequent research. Ultimately, this approach aligns with the FAIR principles (Findable, Accessible, Interoperable, Reproducible), fostering a more robust, collaborative, and reliable data ecosystem.

References

[1] S.Sandlobes et al, Acta Materialia, 2012.

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