Ab-Initio metrics pipeline for the Evaluation of Material Generative Models

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The rapid advancement of generative deep learning models [1-4] has opened new avenues for the discovery of stable materials with targeted properties. However, despite their promising results, evaluating these models remains challenging due to the lack of standardized evaluation methodologies and alignment with chemists' requirements. The most reliable evaluation technique, Density Functional Theory (DFT) simulations, provides accurate assessments of material stability but is computationally expensive and often inaccessible to non-experts. To address this gap, we introduce an easy-to-use and efficient evaluation tool that seamlessly integrates pre-tuned DFT simulations with a diverse set of robust metrics, enabling both chemists and ML practitioners to assess generative models effectively. Our framework performs automated DFT static energy calculations and relaxations, and stability validations against existing material databases through convex hull construction [5], ensuring a rigorous yet accessible evaluation process. By making these complex simulations more user-friendly and computationally feasible, our tool fosters greater collaboration between chemistry and ML communities, accelerating the discovery of novel materials. Our methodology is fully transparent, well documented and open-source, ensuring reproducibility and broader adoption.

References

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Figures

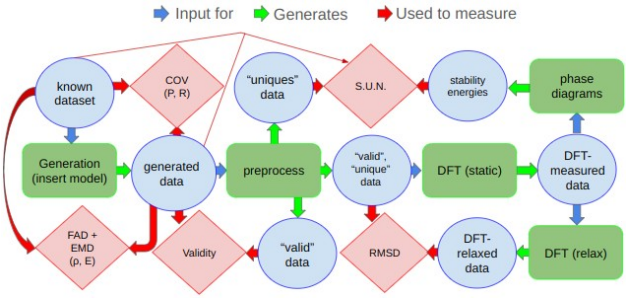

Figure 1. Global overview of the metrics pipeline workflow.