Non-stoichiometric TMDC rapid energy prediction and stable configuration search

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The study of defects in two-dimensional (2D) materials, specifically transition metal dichalcogenides (TMDC) such as molybdenum disulfide (MoS2) and tungsten diselenide (WSe2), is pivotal in the field of materials science. These materials feature a distinctive structure, comprising a plane of metal atoms sandwiched between planes of chalcogen atoms. This layered configuration is crucial in determining its physical and chemical properties. Two-dimensional crystals, particularly transition metal dichalcogenides, have received significant attention due to their unique electronic, optical, and mechanical properties Tedstone et al. [2015], Wang et al. [2012], Han et al. [2015]. The importance of point defects in 2D materials was shown in Koperski et al. [2015].

Density functional theory (DFT) is a primary research method used in materials science. While DFT provides valuable insights, it can be resource-intensive and less effective in predicting properties for materials with high defect densities. This limitation highlights the need for alternative approaches. Machine learning emerges as a promising tool, offering the potential for more efficient and precise predictions of material properties, especially in complex defect scenarios. This shift towards computational methods signifies a crucial step in advancing the study of 2D materials beyond traditional boundaries. Bridging the gap between the recognized importance of studying defects in 2D materials and the limitations of current methods, our study introduces a novel approach. We utilize machine learning, specifically a regression model, to predict the energy states of MoS2 and WSe2 in various defect configurations.

The study presents a novel machine learning method for predicting the energy states of transition metal dichalcogenide within various defect configurations. Leveraging datasets of low and high defect concentrations, the research showcases a regression model that notably surpasses previous energy prediction efforts, achieving an impressive mean absolute error as low as 0.00215 eV for certain datasets, indicating high accuracy and robustness. The approach is highly data-efficient, utilizing only a few samples from specific defect-number classes to predict energy across entire classes of configurations, and performs rapid evaluations via linear regression with minimal features. The study paves the way for practical applications, such as identifying stable atomic configurations, and sets forth a future research direction to explore potential geometric patterns and defect-induced symmetries through density functional theory computations.

References

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Figures

Number of Defects	MAE of our method, Formation Energy Per Site, eV	MAE of MEGNet for Sparse Representation, Formation Energy Per Site, eV
3	**0.0022**	0.004 ± 0.001
4	0.010	
9	0.034	
14	0.036	0.023 ± 0.005
19	0.034	
24	0.039	
Low Density (2, 3)	**0.00215**	0.004 ± 0.001
High Density (4 - 24)	0.031	**0.023 ± 0.005**

Figure 1. Comparison with the State-of-the-Art Method for energy prediction for MoS2.

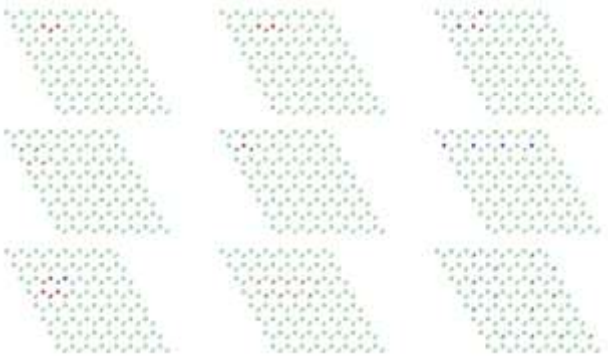

Figure 2. Examples of stable configurations found inside different classes with 4, 9, and 14 defects. Larger points for middle layer atoms; smaller pairs for outer layers. Green shows defect-free areas, red for vacancies, and purple for substitutions.