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# SE(3)-Transformers for predicting the electronic structure of hydrogen molecules

In this work, we demonstrate the efficacy of a neural network model
implemented as the Materials Learning Algorithms (MALA) package
in predicting the electronic structure of a system of hydrogen molecules
under various pressure and temperature conditions across the molecular liquid-solid phase boundary, demonstrating the potential of our
methods for molecular systems. Additionally, we investigate the use
of SE(3)-Transformer Graph Neural Networks to improve the generalizability and extrapolation capabilities of our models. Our results
indicate that the MALA framework provides a powerful and efficient
tool for accelerating Kohn-Sham density functional theory calculations
in molecular systems. This work paves the way for future research in
developing advanced machine-learning algorithms for accelerating electronic structure calculations both accurately and efficiently.

## References

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