PSI Center for Scientific Computing, Theory and Data

Predicting electronic screening for fast Koopmans spectral functionals

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Summary

- Koopmans functionals are a powerful tool for predicting spectral properties of materials (as accurate as state-of-the-art GW)
- However, they rely on electronic screening being captured by "screening parameters"
- We construct a machine-learning model to predict these parameters
- Minimal training data is required

Screening parameters

Insert here a figure of the screening parameters being required (see CECAM talk)

The use-case

Insert here the figure from MARVEL meeting

The model

Descriptors inspired by SOAP descriptors

$\rho_i(\boldsymbol{r}) \rightarrow$

Network simply ridge regression!

Accuracy

- Model predicts screening parameters with high accuracy
- Koopmans functionals with predicted parameters are as accurate as GW
- Model is transferable to new materials

Speed-up

Transferability

References

For more details see Schubert *et al.*, npj Computational Materials (2024)