Quantum-Accurate Multiscale and Data-driven Methods for the Simulation of Materials Failure

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I will describe recent, rapid progress in the development and application of machine learning interatomic potentials (MLIPs) to 'chemomechanical' problems in structural materials that simultaneously require accurate local chemistry and long-range stress fields - e.g. fracture and plasticity. Examples will include the construction of surrogate models for plasticity in tungsten [1], as well as combining two potentials with different accuracy/cost tradeoff choices in different parts of a large system [2]. The recent arrival of foundation MLIP models that leverage large datasets and deep learning have produced models capable of describing much of the periodic table with reasonable accuracy. I will critically assess the applicability of the MACE MP0 and MPA models [3] to chemomechanical problems, and present results from fine-tuning them to improve their (already reasonable) out-of-the-box description of these systems [4]. Finally, I will discuss the importance of robust uncertainty estimates when using these surrogate models and report recent efforts in this direction [5].

References

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[2] F. Birks, T. D. Swinburne and J. R. Kermode, Efficient and Accurate Spatial Mixing of Machine Learned Interatomic Potentials for Materials Science, arXiv:2502.19081 (2025)

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[4] P. Grigorev, F. Birks, T. D. Swinburne and J.R. Kermode, In Prep (2025)

[5] I. R. Best, T. J. Sullivan, and J. R. Kermode, Uncertainty Quantification in Atomistic Simulations of Silicon Using Interatomic Potentials, J. Chem. Phys. 161, 064112 (2024