Contribution ID: **44** Type: **invited**

A foundation model for atomistic materials chemistry

Monday 26 May 2025 11:10 (30 minutes)

The general problem of first principles force fields is to create surrogate models for quantum mechanics that yield the energy of a configuration of atoms in 3D space, as we would find them in reality for materials or molecules. Over the last decade significant advances were made in the attainable accuracy, and today we can model materials and molecules with a per-atom energy accuracy of up to 1 part in 10,000 with a speedup of over a million or more compared to the explicit quantum mechanical calculation, enabling molecular dynamics on large length and time scales. The most surprising aspect of the best model is its extreme generalisation: fitted only on small periodic crystals, it shows stable trajectories on arbitrary chemical systems, from water to nanoparticles and proteins. I will show some of the technical details behind the success of our models: equivariant many-body graph polynomials with very few and weak nonlinearities. The relationship between the architectural elements and the extreme generalisation is still a mystery. The locality of the graph structure is key to its success, as well as high body order and message passing.

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Session Classification: invited