**Towards *ex-machina* computations of transport and transformations in complex materials**

Harnessing the accuracy of quantum mechanics to design complex materials requires a series of approximations to reach the desired length and time scales. I will describe our pursuit of the paradigm of “ex-machina” computations where data-driven approximations are automatically developed using machine learning algorithms and enable access to previously intractable systems. Using non-local charge density descriptors, we trained exchange and correlation density functionals that satisfy exact physical constraints and are competitive with existing semilocal and hybrid empirical functionals. Non-parametric regression methods also allow for learning of potential energy surfaces from expensive quantum calculations. To accelerate molecular dynamics calculations, we developed the Neural equivariant interatomic potential model (NequIP) based on tensor-valued symmetry-preserving layer architectures and used them to achieve state-of-the-art accuracy and training efficiency for simulating dynamics of molecules, liquids, heterogeneous catalysts, and ionic conductors. In order to enable autonomous selection of the training set for reactive systems, we developed the FLARE adaptive closed-loop algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation, using Gaussian process regression. We demonstrate the performance of ML-accelerated MD simulations by studying 2D-to-3D transformations of layered quantum materials, shape memory effect in alloys and thermal transport in semiconductors. Finally, we develop dimensionality reduction techniques in order to automatically identify the reaction coordinates from dynamics simulations, that can be used to enhance sampling of rare transitions and to estimate reaction rates.

**Bio:**

Boris Kozinsky is an Associate Prof. at the Harvard School of Engineering and Applied Sciences. He studied at MIT for his B.S. degrees in Physics, Mathematics, and Electrical Engineering and Computer Science, and received his PhD degree in Physics also from MIT. He then established and led the atomistic computational materials science team at Bosch Research in Cambridge MA, before moving to Harvard in 2018. He works at the intersection of fundamental materials physics, computational methods, and data science. His group develops and uses atomistic and electronic structure computations and machine learning for understanding design rules governing quantum-level microscopic effects, particularly ionic, electronic and thermal transport and transformations in materials for energy storage and conversion. His work on development and application of computational methods led to computation-driven discovery of new materials advances and over 50 patents applications in a wide range of materials systems, including 1D and 2D materials, piezoelectrics, thermoelectrics, batteries, super-ionic conductors, catalysts, and functional polymers. Website: <http://bkoz.seas.harvard.edu>

A person wearing a blue shirt and smiling at the camera

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