



HARVARD
School of Engineering
and Applied Sciences

Computational design of functional materials

Postdoctoral and PhD positions

The newly established Materials Intelligence Research group (<http://bkoz.seas.harvard.edu>) at Harvard School of Engineering and Applied Sciences is seeking postdoctoral fellows and PhD students to join the effort to develop and apply computational methods combining quantum physics with data science to discover new materials for energy and information technologies. We emphasize technological impact and work in close collaboration with leading industrial and academic research groups.

Postdoctoral and PhD projects include:

- Design of materials for next-generation fuel cells and solid-state batteries using computations of electrochemical stability and ionic conductivity of crystals, glasses, polymers and interfaces.
- Machine learning approaches for accelerated materials screening, identifying computable descriptors for ionic and electronic transport properties.
- Development of methods combining first-principles quantum simulations with statistical and physical models of coupling between electrons, phonons and ions, with focus on low-dimensional materials.
- Implementation of database-driven cloud infrastructure for intelligent automation of large computational workflows.

Requirements:

- *Postdocs*: working knowledge of atomistic modeling, including molecular dynamics and quantum mechanical techniques for solid-state and molecular systems.
- Mastery of fundamental solid-state physics, chemistry and transport processes.
- Independence, creativity and strong writing and presentation skills.
- Experience using Python for developing data analysis and automation codes.

PhD candidates should follow the SEAS application process and indicate interest. (<https://www.seas.harvard.edu/audiences/prospective-graduates/apply>)

Postdoctoral candidates should provide as a single pdf: 1-page cover letter, full CV, at most 3 publications, list of 3 references to Boris Kozinsky bkoz@seas.harvard.edu.