

## Quantum design of materials for energy-efficient information and communication technology: abstraction, automation, and machine learning

\*Feliciano Giustino<sup>1,2</sup>

<sup>1</sup>Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, Texas 78712, USA, <sup>2</sup>Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA

\*[fgiustino@oden.utexas.edu](mailto:fgiustino@oden.utexas.edu)

Keywords: Materials design, electronic transport, first-principles simulations, machine learning, 2D materials

If current trends persist, Information and Communication Technology (ICT) could consume nearly 30% of global electricity by 2050, driven by rapid growth in data science, cloud computing, and artificial intelligence (AI). For example, training GPT-4 required an estimated 30 gigawatt-hours of electricity, which is an order of magnitude more than its predecessor. For big data and AI to grow sustainably, a drastic reduction in ICT power consumption is essential.

At the heart of ICT lies the transistor. Two promising strategies to improve its energy efficiency are to reduce operating voltages and to integrate logic with memory. Today's transistors require nearly one volt to switch due to the "Boltzmann tyranny," which limits subthreshold swing. Atomically-thin two-dimensional (2D) semiconductors offer a route to reduce this threshold to the millivolt scale via sharper electronic density of states. Meanwhile, conventional von Neumann architectures incur high energy costs due to the separation of logic and memory. Neuromorphic architectures, where logic and memory are co-located in electrochemical synapses, could reduce the power consumption of a transistor to the level of biological neurons. The success of these strategies critically depends on the discovery and design of new materials.

In computational materials science, we are reaching a tipping point where first-principles quantum simulations can play a transformative role in these areas. To illustrate these advances, I will describe our recent work on the search for high-mobility 2D channel materials for ultrascaled transistors, and on the physics of polarons in oxides for neuromorphic computing. In these applications, there are two relevant transport regimes: diffusive transport, where electrons are delocalized, as in 2D semiconductors like MoS<sub>2</sub>; and hopping transport, where electrons are localized, as in oxides like TiO<sub>2</sub>. For diffusive transport, the key tool is the *ab initio* Boltzmann transport equation, which takes into account the microscopic mechanisms of electron scattering by phonons and defects. For hopping transport, the central challenge is predicting polaron formation, that is the self-trapping of electrons by lattice distortions. These simulations require high-performance computing (HPC) capabilities; in my group we perform these calculations by developing and using the EPW code (<https://epw-code.org/>), an open-source software for first-principles calculations of electron-phonon interactions and related materials properties.

I will also introduce new computational frameworks designed to streamline and automate these calculations, including the MATCSSI cloud integration platform (<https://matcssi.tacc.utexas.edu/>) and the EPWpy abstraction library (<https://epwpy.org/>). MATCSSI is a collaboration between several institutions and the Texas Advanced Computing Center, and provides a cloud portal with interactive Jupyter Notebook support for running advanced electronic structure calculations directly on leadership-class supercomputers. EPWpy, in turn, offers a light-weight interface to define materials and specify complex calculation workflows using an intuitive, high-level Python syntax, and enables automation for high-throughput workflows and machine learning tasks.

These cyberinfrastructure projects aim to lower the barriers to entry for researchers interested in first-principles calculations of transport properties and beyond, promote transparency and reproducibility in materials modeling, and bridge traditional electronic structure methods with modern AI ecosystems for data-driven discovery and AI-accelerated materials design.