**Quantum Design of Materials for Energy-Efficient Information and Communication Technology**

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*Abstract*: The goal of this project is to develop and deploy quantum simulation methods for the design of radically new materials underpinning energy-efficient information and communication technology (ICT). At the current pace, the power consumption by ICT will account for one fifth of global greenhouse gas emissions by 2040. This trend reflects the exponential growth of big data technologies such as data centers, internet of things, cloud computing, machine learning, and artificial intelligence. To enable sustained and sustainable growth of big data in the zettabyte era without compromising climate targets, the power consumption by ICT must be reduced drastically. Disruptive new materials designed for superior energy efficiency will be key enablers in this endeavor. In this project, I will use atomic-scale quantum simulations and massively-parallel supercomputers to create new materials for energy-efficient ICT on an atom-by-atom basis. Quantum simulations have emerged as an extraordinarily powerful tool for designing new materials and predicting their properties with unprecedented precision. To improve and expand the predictive capabilities of current methods, I will develop novel quantum simulation techniques and high-performance computing algorithms for calculating charge transport coefficients of three-dimensional and two-dimensional materials. I will use these new developments to design two-dimensional semiconductors for energy-efficient nanoscale transistors, and oxides for energy-efficient neuromorphic computing via artificial synapses.