

# “Spintronics Preeminent Team Seminar”

April 11, 2016 @ 1:00PM

WANG, 1004

**SPEAKER: Dr. Rajib Rahman**

**Research Assistant Professor, Purdue University**

## **Atomistic Modeling of Nano Devices: From Qubits to Transistors**

**Abstract:** While the end of Moore’s Law marks the end of the glory days of electronic devices, it also opens up opportunities to explore novel concepts in computation and device design. Use of the spin degrees of freedom has attracted much attention in both classical computing and in the emerging field of quantum computing. However, spins at the nanoscale are susceptible to the inhomogeneous local environment of the devices through their coupling to charge and valley degrees of freedom, and to other atoms of magnetic nature. To understand how these atomic scale magnetic interactions manifest in the behavior of devices, atomistic modeling techniques are needed that unify the treatment of spin and charge and provide a description of electronic structure and carrier transport from a fully quantum mechanical standpoint. In this talk, I will describe such a framework that can capture complex interactions ranging from exchange and spin-orbit-valley coupling in spin qubits to non-equilibrium charge transport in tunneling transistors. I will show how atomistic full configuration interaction calculations of exchange in donor qubits help to propose an improved two-qubit gate in silicon. I will also show how spin-orbit-valley coupling due to interface roughness affects the spin resonance frequencies and spin lifetimes in silicon quantum dots. Finally, I will show how atomistic transport simulations help to identify the best 2D materials and designs for tunnel transistors.

**Bio:** Rajib Rahman obtained his PhD degree in Electrical and Computer Engineering from Purdue University in 2009 in the area of computational nanoelectronics. Subsequently, he was a postdoctoral fellow in Sandia National Laboratories in the Silicon Quantum Information Science and Technology group. Since 2012, he has been employed as a Research Assistant Professor in the Network for Computational Nanotechnology (NCN) at Purdue. Rajib develops and employs atomistic simulation methods to model spin qubits in semiconductors taking into account their complex interaction with the environment in the form of electron-electron, electron-phonon, and magnetic interactions. He collaborates with leading experimental groups from Australia, Netherlands, and USA in the field of silicon quantum computing. At Purdue, Rajib also works on atomistic transport simulations of energy efficient transistors in emerging 2D materials.