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First-principles theory on dynamic spin polarization of nuclei in solids

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Nuclear spins weak coupling to external degrees of freedom not only implies long relaxation times, which makes nuclei attractive for quantum bit (qubit) applications, but causes serious difficulties in individual nuclear spin initialization and read-out. Nuclear spin polarization is traditionally achieved by high magnetic field at low temperatures in static processes, which generally give rise to only minor population difference between the different spin states. Dynamic nuclear polarization (DNP) processes, which utilize the coupling of electron and nuclear spins to realize polarization transfer from the easy-to-address electron spin to the nuclear spin, can be implemented by point defect spin qubits in conventional semiconducting material to achieve outstandingly high nuclear spin polarization for a small number of nuclei at room temperatures. Recently, 99 ± 1In my talk, I shortly review the electronic structure and spin Hamiltonian of the most important point defect qubits, discuss first principles techniques for the determination of spin coupling strengths, such as the hyperfine coupling and zero-field-splitting, as well as introduce the model of the dynamic nuclear spin polarization. Through this model, I examine the role of electron state lifetimes and spin relaxation times as well as the possibility of radio-frequency-free bi-directional nuclear spin polarization of distinct nuclear spin for advanced nuclear spin initialization control.