Amorphous nanomaterials in qubits and PCMems: quantum tunneling and thermal transport by first-principles, enhanced sampling and machine learning

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The present Ph.D. project aims at applying advanced computational methods to investigate quantum tunneling and thermal properties of amorphous nanomaterials. This two-fold challenge is of fundamental relevance for applications in quantum computing and phase-change memories (PCMems). The primary objective will be exploiting theoretical and numerical approaches, spanning over first-principles molecular dynamics, enhanced sampling techniques and machine learning, to carefully assess the nature of two-level systems[1,2] (TLs) and the thermal behaviour of amorphous nanomaterials in qubits and PCMems[3]. The detailed microscopic picture provided by these computational studies is prone to deliver fundamental insights into TLSs energy and tunneling landscapes at low temperature. At higher temperature, the outcome will be a comprehension of the nature of the vibrational modes in amorphous materials and the range of the associated mean free paths determining the sensitivity of the thermal properties to down-scaling, a hot topic for a controlled use of disordered materials[4] in PCMems for neuromorphic computing. Tackling these two challenges represents a step forward towards the limitation of qubit decoherence due to TLSs and the engineering of these defects in amorphous materials at the nanoscale. These studies, making use of high-performance computing (HPC) facilities hosted locally, at the HPC centre of the University of Strasbourg (Tier-2 level), and nationally via GENCI (Tier-1 level), will stimulate computer designed experiments where a superconducting quantum device can be employed to study single or multiple TLSs. On a broader perspective, understanding TLSs and their thermal behaviour in amorphous nanomaterials will pave the route to the exploitation of TLSs for hybrid quantum computing[5] where SC qubits or TLSs interact with other quantum systems. A PhD student motivated, with a previous knowledge of quantum mechanics and possibly simulation computer codes (Linux / Unix environment) will represent an ideal candidate for this research project.
Note: Ph.D. project in collaboration with Evelyne Martin (ICube, Équipe MaCÉPV) E-mail: evelyne.martin@unistra.fr

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