Exploration of a 2D Material Monte Carlo Simulator: Parallelization Strategy and Noise Characterization of MoS_2

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ABSTRACT

Two dimensional (2D) metal dichalcogenides are under an intensive research which is mainly motivated by their inherent bandgap and their feasible applications beyond gapless graphene [1]. The dichalcogenides possess fascinating properties such as an atomic-scale thickness and a direct bandgap, promising novel optical and electronic properties [2]. An exhaustive study of electronic transport of these materials is essential to assess their application by advanced physically-based models as an ensemble Monte Carlo (MC) technique which present well-recognised benefits to model the stochastic and quantum-mechanical transport processes at nanoscale.
In this work, an in-house ensemble MC simulator has been developed and widely tested for the study of different 2D materials such as graphene, silicene, molybdenum disulfide (MoS_2) and other transition metal dichalcogenides [3, 4, 5, 6]. We have focused on exploiting the advantages that this tool offers to characterize the microscopic noise sources in MoS_2 due to charge fluctuations. The random stochastic processes of the Monte Carlo method allows us to analyse different fluctuation magnitudes in depth such as the diffusion coefficient, or evaluate the influence of a scattering on the fundamental thermal noise source, which represents a novel approach for the study of noise in these materials.
A parallelization strategy under Message Passage Interface (MPI) has also been employed to upgrade our purely sequential MC simulator, which is essential for diminishing the heavy computational burden of the simulations performed. The motion of simulated particles in the ensemble MC technique depends on their previous history probabilistically govern by Boltzmann Transport Equation using classical free flights interrupted by quantum-mechanical scattering events. This combination of classical and quantum-mechanical probabilities require well balanced approaches to distribute particles to CPU cores in order to achieve balance computer performance [7]. A deep analysis all the particularities of the physical model and the balanced parallelisation approaches has been therefore developed.
The results for analysis of the high-frequency behaviour and the diffusive properties of the electronic transport will be presented for MoS_2 and a decrease in the CPU times of simulations of the 2D materials will be explored.

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