Soutenance de thèse

Vendredi 31 Mai
13h30, Salle A003 - C2N

Monte Carlo simulations of phonon transport in nanostructures based on ab-initio methods

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Jury Members :
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Abstract :
As the trend towards miniaturization of electronic devices continues, understanding heat transport at the nanoscale becomes increasingly crucial for developing energy-efficient and reliable systems. Conventional Fourier's law fails to capture the complex dynamics of phonon-based heat transport in such miniaturized devices. In this thesis, we study the phonon transport within nanostructures employing stochastic Monte Carlo methods. The accuracy of the simulations is enhanced by utilizing full band material description derived from ab-initio calculations based on density functional theory (DFT) without reliance on empirical parameters. We focus on examining alternative materials, such as GaAs, and 2D materials, like graphene, h-BN, and TMDCs, each selected for their unique thermal properties. This work not only offers substantial contributions to the field of thermal transport in nanostructures but also opens new pathways for the design and application of advanced materials in electronics.

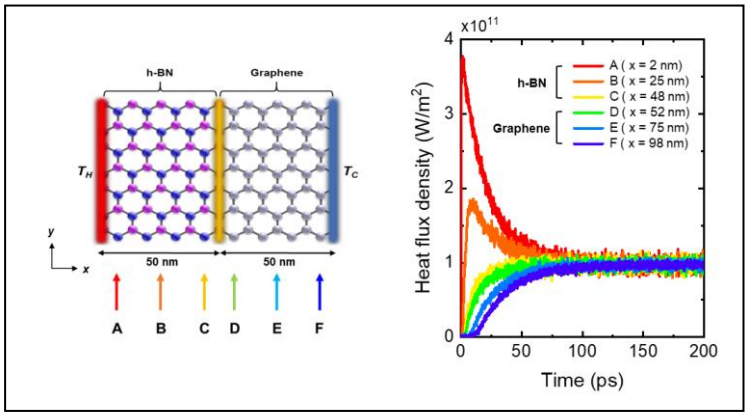

Figure :
- Left grahp : Sketch of the simulated 100 nm 2D h-BN/graphene lateral heterostructure with specific positions (A to F) marked for thermal transient analysis. Positions A, B, C, D, E, and F are located at 2, 25, 48, 52, 75, and 98 nm, respectively, along the x-axis within the structure. Red/blue faces for hot/cold thermostats with TH = 400 K, TC = 300 K, respectively
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- Right graph : Transient heat flux density at 6 points in 100 nm h-BN/graphene lateral heterostructure, measured from 0 to 200 ps. The rainbow color grade intuitively represents the varying heat flux densities according to their respective positions : red for position A, orange for B, yellow for C, green for D, blue for E, and navy for F.