Mathematical Modeling and Numerical Analysis for Incommensurate 2D Materials

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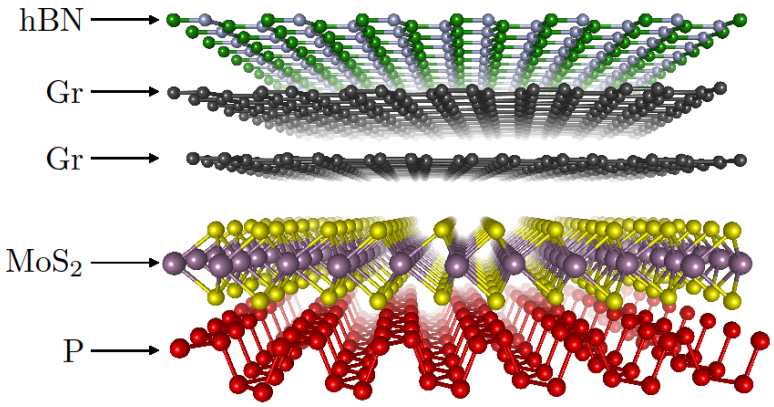
Stacking a few layers of 2D materials such as graphene and molybdenum disulfide, for example, opens the possibility of tuning the electronic and optical properties of 2D materials. One of the main issues encountered in the mathematical and computational modeling of 2D van der Waals heterostructures is that lattice mismatch and rotations between the layers destroys the periodic character of the system.

Basic concepts like mechanical relaxation, electronic density of states, and the Kubo-Greenwood formulas for transport properties will be formulated and analyzed in the incommensurate setting. New computational approaches will be presented and the validity and efficiency of these approximations will be examined from mathematical and numerical analysis perspectives.



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