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Large scale electronic structure calculations of nanosystems on supercomputers LIN-WANG WANG, Lawrence Berkeley National Laboratory — Using linear scaling three dimensional fragment (LS3DF) method, and running on the Oak Ridge Leadership Computing Facility, we have studied the electronic structures of nanoscale systems with tens of thousands of atoms. The LS3DF is a divide-and-conquer method, which divides a large system into many small fragments, and solves each fragment using quantum mechanical methods. The LS3DF method can run on computer like Titan with tens of thousands of cores and on GPU processors. We have studied the electron localization of MoS2/MoSe2 bilayer. Such bilayer forms Moire pattern from the atomic structure point of view. We show that the electronic state can also be localized following such atomic Moire pattern. We have also studied the wave function localization in the hybrid perovskite. We show that, the electrostatic fluctuation caused by the random orientation of organic molecule CH3NH3 is sufficient to localize the electron wave function and significantly reduce its carrier mobility. Finally, we have also studied various nanoscale vortices in a ferroelectric system. Such ferroelectric nanoscale structure can significantly alter the electronic structures of the systems and change their transport properties. This work is supported by BES/SC/DOE, through the Theory of Material program (KC2301) and by INCITE for computer time.

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