Carrier localizations due to nanoscale pattern, ordering and random fluctuations

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In this talk, I will present our recent works in carrier localizations due to nanoscale pattern, ordering and random fluctuations. Linear scaling density functional theory calculations are used to study these phenomena using supercells with thousands or tens of thousands of atoms. The first example is the hole localization due to Moire's pattern in a $MoS_2/MoSe_2$ double layer. We found that the structural Moire's pattern will lead to wave function localization in its electronic structure. The second example is the electronic structure in the ferroelectric nanowire of $BaTiO_3$ embedded in $SrTiO_3$ matrix. The $BaTiO_3$ nanowire can form a ferroelectric vortex, which in turn can change the band alignment type between $BaTiO_3$ and $SrTiO_3$, and also cause charge separation. The nanowire system can also have a skyrmion state, which cause even stronger wave function localization. Lastly, I will present the study on $CH_3NH_3PbI_3$ hybrid perovskite system. We found that the random orientation fluctuation of the CH_3NH_3 molecules will cause strong potential fluctuation in the bulk system, which in term cause carrier localizations. On the other hand, the dynamic nature of the random rotations of the CH_3NH_3 molecules will also cause carrier movement, and is responsible for the carrier mobility of the material