Large Scale Electronic Structure Calculations of Nanosystems using Titan Machine

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In this talk, I will present our ab initio calculations of various types of nanoscale systems ranging from a few thousand atoms to tens of thousands of atoms using Titan machine at OLCF. The systems studied include: (1) the surface passivation of colloidal quantum dot, where an atomistic model of the surface is revealed through ab initio calculations; (2) the defect states of colloidal quantum dots, where it is found that the imperfections of the quantum dot atomic structure do not induce electronic gap states; (3) the Moire's pattern of a bilayer transition metal chalcogenide, where the atomic structure Moire's pattern induce electronic state localizations; (4) the CH3NH3PbI3 hybrid perovskite material, where the random orientations of the organic molecule CH3NH3 induces large electrostatic potential fluctuation, which localizes the electron carriers; (5) the vortices of ferroelectric materials, which causes band alignment changes. All these calculations will be impossible without the use of supercomputers like Titan.