The thermal storage technology based on the use of PCMs has recently raised an important practical interest as it allows the decoupling between production and demand of energy. As rapid development of nano-technology, it has provided new way to thermal energy storage with PCMs. Mesoporous heterogeneous composites are becoming a hot point in nano area. This new type of composites assembled by anisotropic meso-porous substrate and heterogeneous nano-particles/clusters by various means such as ultra-molecular assembly show many distinctive features in optics, electricity, magnetism and heat aspects. Silica-based and non silica-based mesoporous materials are the two common substrates for mesoporous composite materials. The heterogeneous materials which be filled in porous media are some kinds of metal, metal oxide and nano-particles/clusters. In our study, a new PCM composite assembled by mesoporous carbon as substrate and metal nano-particles / clusters as heterogeneous phase change material is simulated for investigating its thermal performance. In order to improve the PCMs thermal properties and optimize material design, the studies focus on theoretical analysis. Molecular Dynamic method is applied to simulate the thermophysical properties: specific heat capacity, melting point, phase change enthalpy and the latent heat. The study on different melting behavior caused by size effect is realized by simulations under different filling volume of nano-particles / clusters. Furthermore, some unusual phase change phenomena happened within the limited space are investigated and discussed. The study is expected to provide theoretical foundation for the research and development of PCMs applied to medium temperature and further to promote its promising application.