Comparison of kinetic and potential energy in annealing process of 2-D and 3-D atomic grid of Krypton by molecular dynamic simulation

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In this study we are dealing with 2-D and 3-D molecular modeling of krypton. A 2-D krypton grid of 20 atoms was produced and settled in a water box. By single point calculations the energy and energy gradient were obtained and the system was optimized by Polak-Ribiere algorithm. In the next step the simulated system was annealed for gaining lower energy minimum, and at last the kinetic and potential energy and temperature diagrams were plotted versus time. Same work as previous was done on the 3-D grid of 100 atoms and the results were compared together. The results show that the energy level depends significantly on the number of atoms and the melting temperatures are different in either case.

Key words: Molecular Dynamics, Single Point Calculations, Kinetic Energy, Potential Energy.

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