THEORETICAL STUDY OF SILVER NANOSTRUCTURES USING GUPTA POTENTIAL

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ABSTRACT

Using Gupta potential silver nanostructures have been studied. The Silver nanowires with icosa structure are found to be most stable among the studied structures. Cohesive energy, Young's Modulus and Shear Modulus values have been computed and comparisons of these values (except Poisson ratio) exceed that of bulk silver. Another striking observation about silver nanostructures is that Young's modulus increases with tube radius whereas shear modulus decreases. This study can give more fundamental understanding of nanoscale machines from atomistic motions and contribute to the design, manufacture and manipulation of nano-devices. The knowledge of the structure and stability of silver nanocrystals is of great importance and to model the silver clusters, we make use of Gupta Potential.

KEYWORDS: Ag structures, U, nearest neighbor distance (b), between two adjacent rings (b'), Young's Modulus (Y), Shear Modulus (G), Poisson's ratio (ν)