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Library of Templates of Virtuall Small Clusters of Ga and In with As, P and V Atoms LIUDMILA POZHAR, Western Kentucky University, Department of Chemistry, Bowling Green, KY 42101 — Electronic energy level computations for small atomic clusters are feasible and provide a foundation for realization of a virtual (i.e., fundamental theory- based, computational) approach to synthesis of sub-nanoscale materials with pre-designed electronic and magnetic properties. In this study the Hartee-Fock (HF) and CI/CAS/MCSCF methods have been used to develop about 20 stable pre-designed and vacuum virtual clusters of Ga and In with As, P and V atoms that provide templates for experimental synthesis of the corresponding clusters in confinement and vacuum. The electronic energy level spectra (ELSs) and spin density distributions (SDDs) of the template clusters reflect influence of clusters' growth conditions, form and composition on formation and structure of their valence and conduction bands, the values of their optic transition energies, and collectivization of their spin density distributions. The ELSs and SDDs of the templates are compared and classified according to their possible use in development of sub-nanostructured materials for electronics, magneto-optics and spintronics.

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