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**Electronic Properties of Small Virtual Clusters of Ga and In with As and P atoms** LIUDMILA POZHAR, Western Kentucky University, Department of Chemistry, Bowling Green, KY 42101, ALAN YEATES, FRANK SZMULOWICZ, WILLIAM MITCHEL, Air Force Research Lab, Materials and Manufacturing Directorate, Wright-Patterson AFB, OH 45433 — The electronic energy level structure (ELS) of several virtually (i.e., fundamental theory-based, computationally) pre-designed stable clusters of Ga, In, As and P atoms is investigated by means of the Hartree-Fock method and compared to that of the corresponding virtual clusters grown in vacuum. The results obtained in the course of this study confirm that the ELS and the direct optical transition energy (OTE) of the clusters are sensitive to manipulations with the covalent radii and cluster composition. Thus, a small displacement (in the range of several hundredths of Angstrom) of atoms in stable pre-designed clusters from their respective positions in vacuum clusters leads to a significant decrease in the OTE and formation of the valence and conduction bands. In agreement with previous results, the OTE for such clusters is in the range of several electron Volts and can be manipulated up to 100% by manipulations with cluster parameters.

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