# Structure of the $In_2O_3$ Molecule in the Free State and in the Crystal

Ulises Miranda,[1] Ilya G. Kaplan,[2] Leonid I. Trakhtenberg [1,3]

[1] Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygina St. 4, Moscow 119991, Russia

[2] Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México,

A.P. 70-360, México, D.F., 04510, México

[3] SSC RF "Karpov Institute of Physical Chemistry", 10 Vorontsovo Pole Str., Moscow, 105064, Russia

**Abstract**

The nanomaterials based on $In_2O_3$ molecules are very important for different physico-chemical processes and applications. They are widely used as catalysts, electrodes and chemical sensors. We present the results of our study of the electronic structure of the $In_2O_3$ molecule in the free state and in the crystal. For the free $In_2O_3$ molecule the geometry of its lowest structures, V-shape and linear, was optimized at the CCSD(T) level, which is the most precise computational method applied up to date to study $In_2O_3$. Using experimental crystallographic data we extracted the geometry of the molecule in the crystal. It was found that it has a zigzag, not symmetric structure and possesses a dipole moment 3.7 times larger than the V-structure of the free molecule. The linear structure due to its symmetry has no dipole moment. According to the Natural Atomic population analysis the chemical structure of the linear $In_2O_3$ can be represented as O=In−O−In=O; the V-shaped molecule has the similar double- and single-bond structure. The construction of small nanoparticles and nanoclusters from "bricks" of $In_2O_3$ with geometry extracted from crystal and their use in practical applications is discussed.