

Molecular Geometry Operating System via Bull! Library

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Abstract: An atomic arrangement in the three-dimensional space, referred here to a molecule for convenience, carries a function determined by its structure where geometry is one of most critical factors. Thus, there are many studies on the geometry of molecule. However, it is hard to find either a unified theory or an engine program for the geometry of molecules. We have been developing a new computational paradigm called "Molecular Geometry (MG)" to better understand the geometry-priority molecular structure in a single, unified theoretical framework based on the Voronoi diagram of spherical atoms, the quasi-triangulation, and the beta-complex. To materialize MG, we have been developing an engine program called "Molecular Geometry Operating System (MGOS)" using the BULL! library with which researchers can easily develop special purpose programs to reason the geometry of molecules by simply calling its API functions. In this talk, we will introduce the MG theory, show the MGOS/BULL! architecture, and illustrate how MGOS can be used to facilitate an easy construction of powerful application program for molecular structure analysis. The proposed MGOS can be used for both the assessment of material properties and design of a new material. The MGOS engine and BULL! library can be freely downloaded from the Voronoi Diagram Research Center at Hanyang University (<http://voronoi.hanyang.ac.kr>).

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