Poster 1

Avogadro - An Advanced Chemical Builder, Visualization and Analysis Program

Geoffrey R. Hutchison

The Avogadro project (www.avogadro.cc) is an open source, advanced molecule editor and visualizer designed for cross-platform use in computational chemistry, molecular modeling, bioinformatics, materials science, and related areas. It offers flexible, high quality rendering, and a powerful plugin architecture. Typical uses include building molecular structures, formatting input files, and analyzing output of a wide variety of computational chemistry packages. Avogadro has been downloaded over 700,000 times world-wide, including translations into over 25 foreign languages.

The Avogadro v2 effort is underway, focusing on dramatic improvements in rendering quality, speed, and reliability. While not all features have been adapted for the new platform, it can interactively render over 2.5 million atoms at 30+ fps on standard laptops. Using this robust framework, we seek to build the best chemical editor and visualization tool, including innovative volumetric rendering, greater extensibility through Python scripting, and smart editing tools.

Poster 2

Pitt Quantum Repository: Exploring Molecules in the Classroom

Ritwik Gupta, Jason Naughton, Joshua Rogan, Geoffrey Hutchison, and Daniel Lambrecht

The Pitt Quantum Repository (www.pqr.pitt.edu) is a project to aid chemistry education among college students. Rather than solely looking at static 2D images, students can get direct hands-on interaction with 3D molecules on smartphones, tablets, and laptops, with computed properties. The repository currently includes over 100,000 species with semiempirical PM7 calculations, including a broad subset of PubChem and common organic and inorganic molecules. This summer, we seek to add more accurate DFT calculations, as well as computed orbital diagrams, vibrational spectra, and more to come.