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Avogadro: Free, Open Source, Cross-Platform Computer Program for Building Molecules and Visualizing Structure MARCUS HANWELL, GEOFFREY HUTCHISON, University of Pittsburgh — The Avogadro project is a free, open source approach to building chemical structures. It has integrated analysis, and three-dimensional visualization capabilities. Avogadro also uses external packages to perform quantum structure calculations. The work presented here illustrates a novel approach to working with the results of quantum calculations by visualizing possible molecular orbitals and allowing the user to select orbitals of interest. The Avogadro program allows the user to prepare new jobs for various quantum codes such as GAMESS-US, Q-Chem, Gaussian and Molpro. Due to the plugin based nature of the Avogadro project many specialized options can be added, such as raytracing the electronic structure of the molecule to produce high quality output, building carbon nanotube structures, or designing solid-state structures. Avogadro is already being used by educators and researchers. Due to the free and open source nature of the project, it can be readily downloaded and used by all students in and out of the classroom. It can also be tailored to particular institutions and/or courses.

Marcus Hanwell
University of Pittsburgh

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