



NWChem Version 4.6

NWChem is a computational chemistry software package enabling researchers to apply theoretical techniques to predict structures, properties, and reactivity of chemical and biological species ranging in size from tens to millions of atoms. Use of the software ranges from understanding biological processes such as membrane interactions with minerals to characterizing important geochemical events to investigating catalytic mechanisms. For the best time-to-solution, NWChem is uniquely tailored to be scalable to thousands of processors.

NWChem Version 4.6 was released on May 24, 2004. The worldwide NWChem community of users requested capabilities for studies of reactive systems and in some cases, collaborated in the development and enhancement of many of the new NWChem functions: coupled-cluster methods, density functional theory (DFT), and Q-HOP. The new functions enable researchers to address scientific questions that are relevant to not only DOE mission areas, but also chemical processes that surround us every day.

Photosynthesis, protein functions, and combustion are just a few of the reactive chemical processes around us. Radical species and energized systems called “excited states” can now be examined using the NWChem coupled-cluster and DFT methods to predict kinetics and thermochemistry of high-temperature reactions such as combustion and to model processes such as photosynthesis and solar cell activity. Q-HOP was designed to examine the transfer of small positively charged particles – protons – in systems composed of several thousand atoms. Proton transfer, or “hopping”, is fundamental in chemical activity and plays a major role in the functions of certain bacteria that can remediate subsurface contaminants by reducing the toxicity of metal waste products.

Within the first week of the release, one hundred scientists downloaded Version 4.6; the total number of user agreements worldwide is nearly a thousand. Available on multiple platforms, NWChem operates on most scientific computer systems, from Mac OSX computers to Linux clusters, SGI and SUN workstations, and IBM SP and Hewlett-Packard supercomputers. Widely used by computational chemists and experimentalists, NWChem is freely available for download.

NWChem was developed at the W.R. Wiley Environmental Molecular Sciences Laboratory. For information, see <http://www.emsl.pnl.gov/docs/nwchem/nwchem.html>.

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