This course introduces some of the many ways in which computers are used in modern chemical research. The main emphasis will be on “molecular modeling” including such topics as electronic structure calculation, molecular mechanics, molecular dynamics and Monte Carlo simulation methods. In lesser detail, chemical informatics will also be considered, time permitting. Discussion of the theoretical underpinnings of these various methods and their range of applicability will be combined with exercises illustrating the use of several current chemical software packages and with assignments based on critical reading of illustrative literature papers.
In order to express this idea of chemical union in symbols I would suggest the use of a colon, or two dots arranged in some other manner, to represent the two electrons which act as the connecting links between the two atoms. Thus we may write Cl₂ as Cl : Cl. If in certain cases we wish to show that one atom in the molecule is on the average negatively charged we may bring the colon nearer to the negative element. Thus we may write Na : I, and I : Cl. Different spacings to represent different degrees of polarity can of course be more freely employed at a blackboard than in type.

\[
\left\{- \frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) + V \right\} \Psi(\vec{r}, t) = i\hbar \frac{\partial \Psi}{\partial t}
\]

"The underlying physical laws necessary for the mathematical theory of ... chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

[P. A. M. Dirac, 1929]
Gordon Moore made his famous observation in 1965, just four years after the first planar integrated circuit was discovered. The press called it "Moore's Law" and the name has stuck. In his original paper, Moore observed an exponential growth in the number of transistors per integrated circuit and predicted that this trend would continue. Through Intel's relentless technology advances, Moore's Law, the doubling of transistors every couple of years, has been maintained, and still holds true today. Intel expects that it will continue at least through the end of this decade. The mission of Intel's technology development team is to continue to break down barriers to Moore's Law.

http://www.intel.com/research/silicon/mooreslaw.htm
from: talk by G. E. Moore,
No Exponential is Forever ...
but We Can Delay ‘Forever’,
presented at ISSC Meeting,
Feb. 2003

Processor Performance
MIPS

τ(10) ~ 6 years
τ(2) ~ 2 years
Some examples of the sorts of molecular graphics available today; rendered with the “chimera” program (UCSF)

http://www.cgl.ucsf.edu/chimera/ImageGallery/