CHEM 408: Computer Applications in Chemistry (Really Molecular Modeling)

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Please take a copy of the handouts and begin filling out the Preliminary Survey.
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]
from: talk by G. E. Moore, 
No Exponential is Forever ... but We Can Delay ‘Forever’, 
presented at ISSC Meeting, 
Feb. 2003

\[ \tau(10) \sim 6 \text{ years} \]
\[ \tau(2) \sim 2 \text{ years} \]
Some examples of the sorts of molecular graphics available today; rendered with the “chimera” program (UCSF)

http://www.cgl.ucsf.edu/chimera/ImageGallery/
The “Guided Inquiry” Format

Motivation:

• lecturing relatively ineffective
• exploration, concept formation, application real pattern of learning
• verbalization is a key ingredient, cooperative approach helpful
• teamwork essential process skill beyond content

Class Time Breakdown:

• reading before class (essential)
• ~5 minutes orientation, announcements, etc.
• ~50 minutes teams work on worksheets (25+25)
• ~20 minutes class discussion (10+10)
Team Member Roles:

1. **Manager**: actively participates, keeps team on task, assures that all team members participate and understand.
2. **Recorder**: actively participates, records solutions as worked out by the team for submission.
3. **Speaker**: actively participates, is responsible for describing the team’s work during class discussions.
4. **Analyst**: actively participates, is responsible for assessing the performance of the team and providing feedback on the course work.

- I will choose initial teams based on your survey responses.
- Teams membership will change roughly every month.
- Roles will rotate every class period via cyclic permutation (1→2→3→4→1).