**Applied Theoretical/Computational Chemistry Workflow**

- **Build a starting geometry for a single minimum**
- **Build starting geometries for multiple conformers**
- **Build starting geometry for a transition state structure**

- **Convert to input file for QM software**

- **Run QM calculation (energy, geometry, frequency, property)**

- **Repeat the process**
run QM calculation (energy, geometry, frequency, property)

retrieve information (structural, molecular properties) from text output file

convert atomic coordinate in output file to input file for 3D printer

"print" 3D model corresponding to computed molecular geometry

clean/preserve model for tactile examination

"Computational Chemistry for the Blind and Visually Impaired"

"Visually Impaired Researchers Get their Hands on Quantum Chemistry; Application to a Computational Study on the Isomerization of a Sterol"
AsteriX
Gert Vriend
Valere Lounnas
<table>
<thead>
<tr>
<th>Haptic atom types and corresponding elements in Mendeleev’s periodic table</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Simple spheres</strong></td>
</tr>
<tr>
<td>size: small = [H,D,T]; medium = [C]; large = [Si]; very large = [all other metalloids]</td>
</tr>
<tr>
<td><strong>Icosahedrons covered with small cylinders at corners</strong></td>
</tr>
<tr>
<td>size: small = [F]; medium = [Cl]; large = [Br]; very large = [I,At]</td>
</tr>
<tr>
<td><strong>Simple spheres covered with small spheres</strong></td>
</tr>
<tr>
<td>size: medium (N); large (P)</td>
</tr>
<tr>
<td><strong>Icosahedrons covered with cylinders on facets</strong></td>
</tr>
<tr>
<td>Alkali and alkaline-earth metals</td>
</tr>
<tr>
<td>Size: medium = [Li, Be]; large = [Na, Mg]; very large = [K, Ca, all other ones]</td>
</tr>
<tr>
<td><strong>Simple spheres covered with small cylinders</strong></td>
</tr>
<tr>
<td>size: medium (O); large (S)</td>
</tr>
<tr>
<td><strong>Icosahedrons covered with cylinders on facets</strong></td>
</tr>
<tr>
<td>Transition metals</td>
</tr>
<tr>
<td>size: medium = [4th row]; large = [5th row]; very large = [6th row]</td>
</tr>
<tr>
<td><strong>Simple icosahedrons</strong></td>
</tr>
<tr>
<td>size: medium = [dummy atom type, lanthanides, actinides, any other not otherwise defined element]</td>
</tr>
<tr>
<td>Cross section</td>
</tr>
<tr>
<td>---------------</td>
</tr>
<tr>
<td>Dodecahedron</td>
</tr>
<tr>
<td>Hexagon</td>
</tr>
<tr>
<td>Square</td>
</tr>
</tbody>
</table>

Simplified Braille cipher signs used to emboss bond-length on the surface of the bonds. Only the upper part of the (3,2) dot matrices are used to encode ciphers.
AsteriX
Gert Vriend
Valere Lounnas
Applied Theoretical/Computational Chemistry

**Workflow**

1. **Build a starting geometry for a single minimum**
   - Convert to input file for QM software
   - Run QM calculation (energy, geometry, frequency, property)
   - Retrieve information (structural, molecular properties)

2. **Build starting geometries for multiple conformers**
   - Convert atomic coordinate in output file to input file for 3D printer

3. **Build starting geometry for a transition state structure**
   - Software modifications to improve accessibility

4. **Build tactile model of starting geometry using specialized "printed" parts**
   - "Scan" tactile model into a set of atomic coordinates
retrieve information (structural, molecular properties) from text output file

convert atomic coordinate in output file to input file for 3D printer

"print" 3D model corresponding to computed molecular geometry

clean/preserve model for tactile examination

software modifications to improve accessibility

print in ABS plastic to make cleaning/preservation accessible and improve durability
437 - Nobody can see atoms: Science camps highlighting approaches to making chemistry accessible to blind and visually-impaired students

Authors: Henry B. Wedler, Mrs. Lee Boyes, Dr. Rebecca Davis, Mr. Dan Flinn, Dr. Annaliese K. Franz, Dr. Christian S. Hamann, Dr. Jason G. Harrison, Dr. Michael W. Lodewy, Dr. Christin A Milinkevich, Prof. Jared T. Shaw, Prof. Dean J. Tantillo, Dr. Selina C. Wang

Division: CHED: Division of Chemical Education

Date/Time: Wednesday, August 13, 2014 - 09:45 AM

Session Info: Reaching Out: Chemistry Outreach Programs for High School and Community College Students (08:30 AM - 12:00 PM)

875 - Isomerization of cycloartanol: An indicator of thermally-treated olive oil

Authors: Henry B. Wedler, Ryan P. Pemberton, Dr. Selina C. Wang, Prof. Dean J. Tantillo

Division: ORGN: Division of Organic Chemistry

Date/Time: Wednesday, August 13, 2014 - 01:20 PM

Session Info: Physical Organic Chemistry (01:00 PM - 04:00 PM)
The Goal...

- make applied theoretical chemistry fully accessible to one lacking sight

...idea
...experimental design
...implementation
...results retrieval
...interpretation
...presentation