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Touching the invisible - molecular haptics

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Abstract

Novel, simple, cost-effective applications combining haptics and computer graphics for the study of key chemical concepts such as reactivity and periodicity at AS/A-level and undergraduate level are described.

Categories and Subject Descriptors (according to ACM CCS): H.5.2 [Information Interfaces and Presentation (e.g., HCI)]: Graphical User Interfaces, Haptic I/O; J.2 [Physical Sciences and Engineering]: Chemistry

1. Introduction

Haptics couples the sense of touch with a computer-generated scene and is often employed within immersive environments, where haptics enhances [FPB77] 3D perception from single-/multiple-viewpoint active, passive or autosterescopic technologies. Haptics can be divided into:

- *force (kinesthetic) feedback* - perceptions of resistive forces via robotic manipulators
- *tactile feedback* - perceptions of heat, pressure & texture, e.g. finger tip (135 sensors / cm^2, senses vibrations < 10 kHz, most sensitive at ≈ 230 Hz [BC94])

Currently there are several commercial solutions available for force feedback, but little for tactile feedback.

Table 1: *Commerical Force-Feedback Haptic Devices*

Device	Cost (£*k*)
Haption Virtuose	75
Sensable Phantom Premium	35-55
Force Dimension Delta	28-52
Force Dimension Omega	18-30
Immersion CyberTouch (Tactile) / CyberGrasp	>20
Sensable Phantom Desktop	10
Sensable Phantom Omni	2
Novint Falcon	0.2

Table 1 (non-exhaustive) lists a selection of commercial haptics devices. Note that the price ranges from £200-£75,000 and largely depends on the build quality and degrees of freedom supported. The Novint Falcon utilised in this work, retails for ≈ £200 and can therefore be easily afforded and integrated within a classroom environment.

Affordable graphics with clear educational benefits [CS04] can be obtained by using Web3D technologies such as iso-standard X3D & VRML97. Our hypothesis is that these benefits, which include knowledge-building experiences and the ability to analyze phenomena from different points of view, will help an undergraduate chemistry student to more quickly learn and understand key chemical concepts.

Although a majority of educational haptic applications are used to train surgeons [JRP*01], however, the use of haptics to describe complex molecular and physical phenomena is now becoming more prevalent. Improved perception of a virtual molecule can be obtained via cooperative deconvolution and interpretation of multiple cues - synaesthesia [DUR05].

The first documented haptic interface for scientific visualization was Project Grope [OYPH*88] which allowed perception of force fields, e.g. for molecular docking [ZGAB09]. A molecular surface can be *felt* using the probe tip of an atomic force microscope, whilst nanomanipulators [GF*00] (based upon an identical principle), allow strategic placement of atoms onto thin films, allowing quantum phenomena e.g. quantum dots & corrals to be studied. Force-feedback haptics can be merged with tactile responses from prototyped models [SBO*95, GSSO06] to provide an intuitive learning interface.

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2. Applications

2.1. Molecular Perception

In this section we explore several areas from a typical chemistry syllabus where we believe added value can be gained from using our combination of haptics and computer graphics technologies. Physical molecular models have allowed chemists for centuries to describe complex chemical processes and structures. The pioneering work of:

- Dalton (atoms)
- Loschmidt (2D diagrams)
- Hofmann (first physical model)
- van't Hoff and le Bel (sterochemistry)
- Corey, Pauling & Koltun (CPK space filling models)
- Watson and Crick (DNA)

laid solid foundations for modern molecular graphics & 3D rapid prototyping technologies.

Aesthetic molecular models act as pedagogic tools for students. Although molecular graphics has mostly replaced physical models, the cheapness of the latter, combined with immediate visual & tactile cues, and ease of interaction (e.g. for conformational analysis & pseudorotation) are quintessential to cost-effective haptic applications.

H3D API is an open source, cross-platform, haptics device independent software development platform that employs OpenGL & X3D with haptics to generate a unified scene graph capable of handling haptics, (stereo)graphics & audio. A CPK scheme was employed for atomic rendering, due to scene graph simplicity [DJ*05,Dav07], although halftone cylindrical (and other models) can also be used.

Prototype H3D interfaces are presented which enable probing of key quantum & molecular properties encountered within a Chemistry curriculum.

2.2. Reactivity

The bond energy, E, of a molecule is a measure of the strength of a chemical bond; the latter being related to the bond length & order (Table 2). Although a Morse potential, $E = D_e(1 - e^{-a(r-r_0)})^2$, correctly (bond breaking, unbound states, anharmonicity & transition probabilities for overtone & combination bands) describes the potential energy of a diatomic, a simpler harmonic oscillator model, $E = k(r - r_0)^2$, where k is the force constant (stiffness), & r_0 is the reference bond length was employed.

An initial haptic reactivity model (summarised in the below H3D code) was built for HX (X = F, Cl, Br, I) (Figure 1) in which a single white H atom acts as a haptics probe. A harmonic spring described using a *SpringEffect* haptics node (Table 3) was attached to each atom and displaced vertically to ensure the correct equilibrium bond length. Force constants within the springConstant field were scaled (optimum=100-500) ensuring that force-feeback is neither too weak nor too strong.

```
<X3D>
  <IMPORT inlineDEF='H3D\_EXPORTS'
      exportedDEF='HDEV' AS='HDEV'/>
  <Scene>
    <Group>
    group translation, scaling etc.
    <Transform DEF='H'>
      <Shape>
        <Appearance>
          <Material diffuseColor='1 1 1'/>
        </Appearance>
        <Sphere radius='0.012'/>
      </Shape>
      </Transform>
      other atoms placed here
    </Group>
    <SpringEffect DEF='F' escapeDistance='0.02'
        position='-0.09 0.0092 0'
        springConstant = '483'
        startDistance=0.02'/>
    other springs placed here
    <ROUTE fromNode='HDEV'
        fromField='trackerPosition'
        toNode='H' toField='translation'/>
  </Scene>
</X3D>
```

Table 2: *Example Bond Energies*

Bond	C-C	C=C	C≡C
Bond Energy (kJ mol^{-1})	348	614	839
Bond Length (pm)	154	134	120
Bond Order	1	2	3

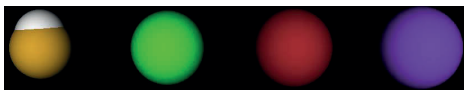

Figure 1: *Reactivity Graphical User Interface*

Table 3: *Harmonic Springs in HX [Lad08]*

Molecule	H-F	H-Cl	H-Br	H-I
$k(Nm^{-1})$	966	516	412	314
r_0 (Å)	0.0927	0.1274	0.1414	0.1609
$D_0(kJmol^{-1})$	565	431	366	299

A class of 54 sophomores were invited to test the effectiveness of the haptics experiment, with 80% correctly identifying the strongest (H-F) and weakest (H-I) bonds. Since the harmonic oscillator is not taught until the second year, direct comparison with traditional educational methods is difficult. An improved interface has been constructed which is now capable of showing (or hiding) values of the force

constants. Nevertheless, subsequent demonstrations for secondary school teachers and their students reveal substantial interest in this novel way of teaching reactivity.

2.3. Periodicity

One of the foremost challenging subjects within the Chemistry curriculum is quantum mechanics and the subtle nuances it plays upon the chemical & physical properties of the elements within the Periodic Table.

2.3.1. Ionization Potentials & Electron Affinities

The n^{th} ionization potential, IP, is the energy required to strip it of the n^{th} electron after the first $n-1$ electrons have been removed, and is an excellent indicator of reactivity. The electron affinity, EA, is the energy released when removing an electron from a singly charged negative ion, i.e. $X^- \rightarrow X + e^-$, although the older convention, $X + e^- \rightarrow X^-$ (opposite sign) is also employed.

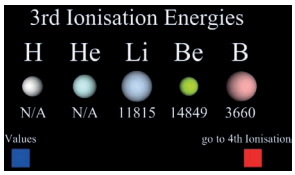

Figure 2: *Ionization Potential User Interface*

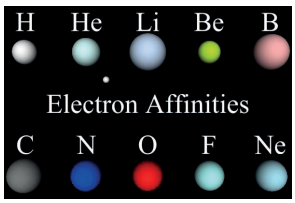

Figure 3: *Electron Affinity User Interface*

Two prototype user interfaces (Figures 2 and 3) consisting of a series of sequential CPK atoms with a harmonic spring described using a *SpringEffect* node attached to the nucleus, and a small haptic probe representing an electron were constructed. In both applications, the user was encouraged to pull the haptic probe representing the electron away from the atom - the spring stiffness (*springConstant* field) representing the magnitude of the IP (Table 4) or EA (Table 5). A logarithmic scaling was employed for the IPs (due to exponential growth for successive IPs), whereas a linear scaling was utilised for EAs, ensuring that the *springConstant* field lay between 100-500 for optimum force-feedback. Although only demonstrated to a small group of secondary school teachers, we envisage that students via a constructed lesson plan, will be able to *feel* trends within the 1^{st} and 2^{nd} IPs, enabling qualitative predictions for 3^{rd}, 4^{th} & 5^{th} IPs.

Table 4: *Selected Ionization Potentials ($kJmol^{-1}$) [Har84]*

Element	1st	2nd	3rd	4th	5th
H	1312				
He	2372	5251			
Li	520	7298	11815		
Be	900	1757	14849	21007	
B	801	2427	3660	25026	32828

Table 5: *Selected Electron Affinities [HKK97]*

Element	H	He	Li	Be	B
EA ($kJmol^{-1}$)	71.8		59.6		26.7

Element	C	N	O	F	Ne
EA ($kJmol^{-1}$)	153.9	7	141	328	

2.3.2. Electronegativity

Electronegativity, χ, is the ability of an atom to attract electron density towards itself within a covalent bond, and correlates with a number of other chemical properties, e.g. IR stretching frequencies, NMR chemical shifts and isomer shifts in Mössbauer spectroscopy. Electronegativity cannot be measured directly, and is calculated from other atomic / molecular properties, e.g.:

- Pauling (A-A, A-B & B-B bond energies) [Pau32]
- Mulliken / Absolute (mean of IP and EA) [Mul34, Mul35]
- others: [AR58, San83, All89]

Discussion of bond polarity relies upon χ, with ionic bonds being formed if $\Delta\chi \gg 0$. By placing haptic springs with *springConstant* values $\propto \chi$, the effects of bond polarity can be haptically described. For ionic Na^+Cl^-, only two springs are felt, whilst an additional (non-scripted) haptic minimum can be *felt* in the middle of the Cl-Cl bond for non-polar Cl_2 (Figure 4). With increasing polarity, the minimum increases towards the halogen (Figure 5).

Figure 4: *Effect of polarity: NaCl (ionic, left), HCl (polar, covalent, middle), Cl_2 (non-polar, covalent, right)*

3. Future Work

Initial proof-of-concept methodologies are presented herein. Completed user interfaces will be demonstrated to lecturers, teachers and students allowing a thorough evaluation of the effectiveness (and any subsequent modification) of the

Figure 5: *Electronegativity in HX: HF(top) to HI (bottom)*

haptic user interfaces. Lesson plans adapted for both university and secondary level will also be created to guage the benefits of the haptic approach over standard teaching methodologies. The extensibility and ease of programming of H3D/X3D will also allow the rapid development of a bilingual (Welsh / English) user interface.

4. Conclusions

Two different approaches for the preparation of novel, simple, cost-effective molecular haptic applications based upon a H3D viewer and a Novint Falcon have been developed which will enable, via suitable lesson plans, which are currently in development, the hands-on demonstration of key chemical concepts taught at both secondary school and undergraduate level, such as reacitivity, periodicity and acidity. Although only a limited number of prototype user interfaces have been evaluated, initial results which seem to favour pupils with high practical aptitudes are encouraging, with lecturers, teachers and students vocalising their support.

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