**m45.o02**

## Teaching three-dimensionality and quantum chemistry by a concerted use of structural databases and of computational and molecular graphic tools

Marco Milanesio[a], Gianluca Croce[a], Piero Ugliengo[b]

*[a] DiSTA, Univ. Piemonte Orientale, Alessandria, Italy; [b] Dip. Chimica IFM, Univ. Torino, Italy.*

**Keywords: computer-aided crystallographic teaching, molecular graphics, quantum chemistry**

Showing students that chemical compounds, are three-dimensional (3D) entities governed by their quantum wave function is a challenging task. It is indeed easier to think of molecules in terms of formulae in chemical equations or 2D sketchs or to consider families of compounds with common properties. Introducing quantum mechanic concepts and demonstrating that quantum chemistry (QC) is a fundamental branch of modern chemistry is a more difficult task. Currently available search engines for structural databases like the CSD[1] suite of programs and molecular graphic tools like Moldraw[2], may be very useful to overcome these difficulties. In fact these softwares allow to set up computer aided exercises, during which students learn: i*)* to search structural databases; *ii)* to graphically inspect the downloaded structures with specific properties; *iii)* to build simple molecules and calculate physical properties related to experiments carried out in other lab courses. The following examples will be illustrated. ***Chemistry****:* the heat of combustion of naphthalene and camphor and the IR spectra of aromatic compounds (benzene, pyridine etc.), experimentally measured in other lab courses, are calculated by employing a QC program, after building the 3D models and the input to the QC program with the aid of structural databases and of Moldraw. In one shot students learn that *i)* molecules are 3D entities and *ii)* QC is a tool able to predict *real* chemical-physical properties. ***Materials Science***: $CuHgI_4$ undergoes a phase transition at 330 K from a low T phase with electric insulator behavior to a high T one acting as an ionic conductor. It can be easily synthesized in a materials chemistry lab, where conductivity experiments can be carried out. By searching and graphically inspecting the crystal structures of the two phases the students can learn that physical properties are related to structural features. ***Biochemistry***: the relationships between the behavior of biological molecules or assemblies (proteins, DNA filaments, anti-tumor drugs etc.) and their 3D structure can be highlighted by stimulating students to search the Protein Data Bank (PDB) [3] for crystal structures related to metabolic pathways, studied in other courses with a ″2D approach″. Typical ″greatest hits″ are normal and mutated hemoglobin, DNA-binding proteins, membrane channel proteins and toxins.

[1] http://www.ccdc.cam.ac.uk
[2] http://www.moldraw.unito.it
[3] http://www.rcsb.org

**m45.o03**

## The STaRBURSTT - CyberInstrumentation Consortium - CyberEnabled Crystallographic Education

A.D. Hunter[a], M. Zeller[a], T.R. Wagner[a]; M. Bond [b], R.J. Butcher[c], G. Crundwell[d], G.M. Ferrence[e], K. Kantardjieff[f], L. Ramirez[g], T. Higgins[h], P. Szalay[i]

*a) Department of Chemistry, Youngstown State University, One University Plaza, Youngstown OH 44555-3663,U.S.A., b) South East Missouri State-University, c) Howard University, Washington D.C., d) Central Connecticut State University, e) Illionois State University, f) California State University Fullerton, g) East Los Angeles College, h) Harold Washington College, City Colleges of Chicago, i) Muskingum College, OH*

**Keywords: instrumentation control, cyberInstrumentation, STaRBURSTT**

The STaRBURSTT-CDC (i.e., *S*cience *T*eaching *a*nd *R*esearch *B*rings *U*ndergraduate *R*esearch *S*trengths *T*hrough *T*echnology - Cyber*D*iffraction *C*onsortium) is a US based consortium made up primarily of Predominantly Undergraduate Institutions, Historically Black Colleges and Universities, and Hispanic Serving Institutions having strong interests in X-ray diffraction. [1] Five core instrumentation hubs at California State University Fullerton, Central Connecticut State University, Illinois State University, South East Missouri, and Youngstown State University are remotely accessible to our 50+ PUI collaborators. This poster will emphasize a range of new curriculum materials developed and tested by this group, including: computer labs on structure determination, local and remote access labs for unknown structure determination, and mini- and full scale student research projects including writing and evaluating of crystallographic papers/publications by undergraduate students. The collection of crystallographic data remotely over the internet will be emphasized. [2]

[1] http://www.starburstt.org/
[2] Paul S. Szalay, Allen D. Hunter, Matthias Zeller. *J. Chem. Ed.* 2005, *82*(10), 1555-1557.