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## Novel Educational Computational Chemistry Learning Environments Effect on Preservice Chemistry Teachers' Perceptions of Technological Pedagogical Content Knowledge

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# NOVEL EDUCATIONAL COMPUTATIONAL CHEMISTRY LEARNING ENVIRONMENTS EFFECT ON PRE-SERVICE CHEMISTRY TEACHERS' PERCEPTIONS OF TECHNOLOGICAL PEDAGOGICAL CONTENT KNOWLEDGE

*The Intermolecular Forces module was designed and implemented on third year undergraduate students of degree in Chemical Education and Pedagogy in Chemistry. This module was designed based on educational computational chemistry model in the technological pedagogical content knowledge framework, to promote learning of intermolecular forces and development of scientific skills in the formal training of pre-service chemistry teachers. A perception study was completed indicating that the students' assessment of the integration of computational chemistry as a tool to aid in the learning of concepts and development of activities with molecular 3D visualization and process models at the molecular scale is positive in terms of content learning associated with intermolecular forces, scientific skills development and perspective professional*

*Keywords:* TPACK, Computational Chemistry and Pre-service Chemistry teacher

## INTRODUCTION

It is difficult to imagine the progress of science without the use of instruments and computers. Specialized software has facilitated processing and analysis of data and contributed greatly to understand scientific phenomena through visual representations. Computational science viewed as the intersection of applied mathematics, computer science, and application sciences (Yasar & Landau, 2003) is intrinsic to chemistry research. In this regard, Computational Chemistry (CC) is the field of chemistry that uses mathematical algorithms, statistics, and large databases to integrate chemical theory and modelling with experimental observations. Today, advances in computer visualization capabilities make possible to show complex analyses in an easily understandable form. These are usually used to design experiments and new materials and to validate the results. Therefore, CC arises as a key area with interesting potential for the mediation of teaching-learning process of chemistry into various levels of formal chemistry education. This work reports on the integration of Computational Chemistry into curriculum of Pre-service Chemistry Teachers' by mean of an Educational Computational Chemistry (ECC) module, a learning environments built on the theoretical principles of the Technological pedagogical content knowledge (TPACK) framework proposed by Mishra & Koehler (2006, 2009) and the use of student-centered pedagogy.(Koehler & Mishra, 2009; Mishra & Koehler, 2006) On this regards, the purpose of this paper was to explore the students' perceptions of novel ECC learning environments through designed learning module, into the TPACK framework. The most relevant aspects, for the participants, of the module implementation were included. Besides, participants' representations of some TPACK components are shown and their prospective perceptions to integrate computational chemistry practices in a pedagogical way in the classroom. In this context, the following research question was directed the study: What are the perceptions of pre-service chemistry teachers after the implementation of a novel ECC learning environment, based on the principles of the TPACK framework?

### **ECC module in the framework of Technological Pedagogical Science Knowledge (TPASK)**

TPACK is defined as "a class of knowledge that is central to teachers' work with technology. This knowledge would typically be held by technologically proficient subject matter experts, or by technologists who know little of the subject or of pedagogy, or by teachers who know little of that subject or about technology" (Mishra & Koehler, 2006). In the case of science education, (Jimoyiannis, 2010) argue that TPASK represents a class of knowledge needed by science teachers to allow productive technology

integration in science education. Consequently, CC integration into pre-service chemistry teachers' education and to support to in-service chemistry teacher constitutes an important basis for teaching chemistry with technology that is proper to the discipline.

Chemistry education and science education are privileged subject matter for the technology integration due to implicit technology development in science. Thus, technology integration can be able to help teachers to provide a learning environment that encourages the development of student-centred learning environments by requiring students to learn independently. (Agapova O.I., Jones L.L., Ushakov A.S., Ratcliffe A.E., & Varanka M.A., 2002) The integration of emerging technologies in science education requires the contextualization of knowledge of these new technologies, considering its use in the generation of scientific knowledge in science and also its social projection. In this regards, the advances in computational methods in chemistry (or CC) represent an example of emerging technology in science that can be used in the teaching of chemistry. The contextualization of this emerging technology in the teaching of chemistry is related to the use of real world problems (RWP) in science and examples of scientific development.

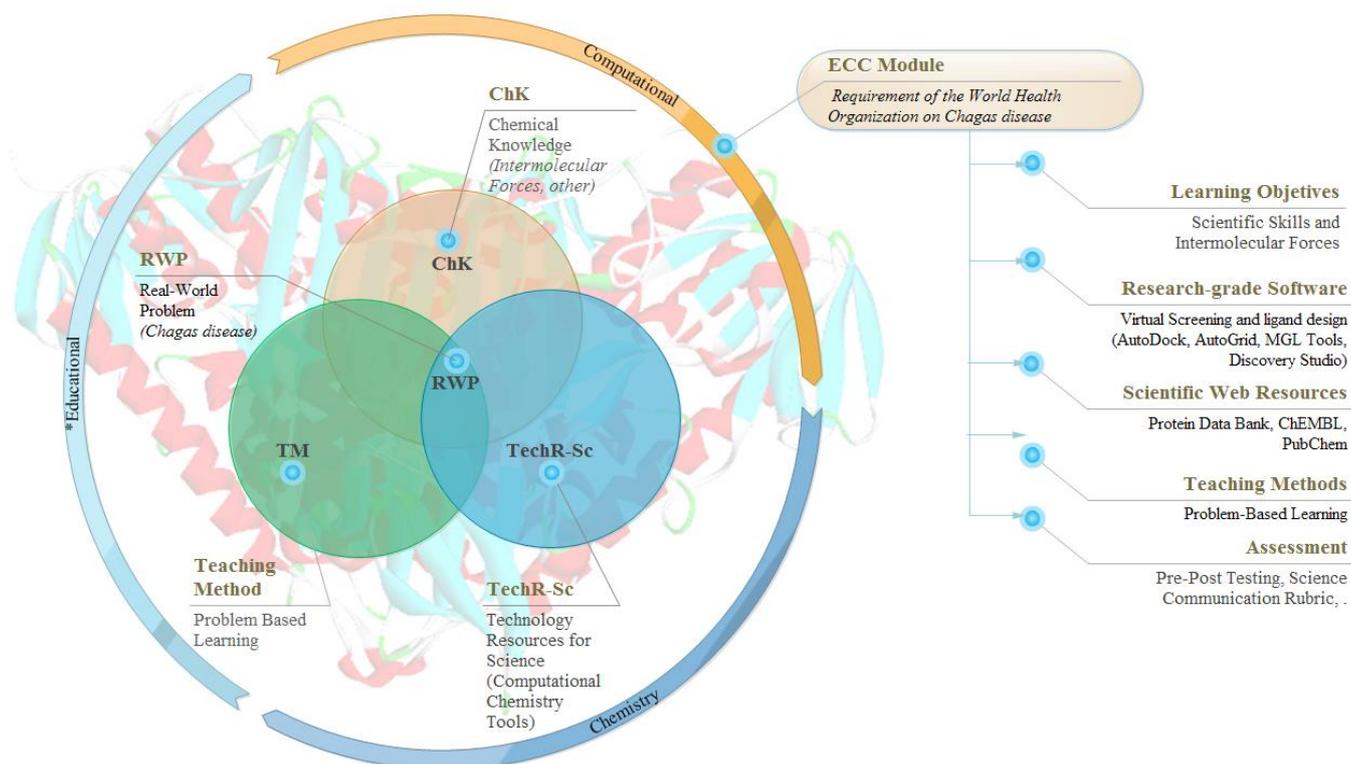
An attempt to integrate computational chemistry and the contextualized chemistry teaching, using a RWP in science with social and environmental projection, we have developed an ECC module (Scheme 1), which expect to: (a) promote the learning of chemical concepts, allowing students to establish their learning needs and priorities; (b) promote meaningful and contextualized learning of chemical concepts based on a RWP in science that integrate the computational chemistry with knowledge of other areas of science; (c) promote the analysis of the approximations used in the models used in CC, delimiting their applicability in a RWP in science. The ECC module can be identify as a practical model that reveal the affordances of the computational chemistry as a knowledge that integrate the technological knowledge of emerging technologies and chemistry knowledge, thus constituting technology chemistry knowledge (TSK). This module shows how the CC can be used with the teaching method of Problem-Based Learning (PBL), considering the chemistry topics specific that the pre-service chemistry teachers will be to teach.

## **METHOD**

### **Design of ECC module and Perception study**

The learning activities described here were part of a module of a regular physical chemistry course. The number of students was 16, which were divided in two groups. Group 1 included six students and group 2 ten. Both groups were monitored by a coordinating teacher. Next, these groups were organised into smaller groups of 2–3 participants. The students' developed the module activities following the steps described previously for the method of Problem Based Learning. The intermolecular forces theme was covered by one PBL scenario for 4 weeks. The PBL scenario: "Requirement of the World Health Organization on Chagas disease", was introduced to the students using one-page consisting of a short descriptive text, which pose the challenge: Identify a potential trypanothione reductase inhibitor among commercially available  $\beta$ -carboline derivatives, using as substructure the  $\beta$ -CD: 1-{1-methyl-9H-pyrido[3,4-b] indol-3-yl}ethan-1-one.

For the perception study a qualitative descriptive design using focus groups method was selected. This method is suited for this research study since we are primarily interested in the perspectives of students regarding of a novel ECC learning environment. This methodological approach was deemed the most suitable for collect qualitative data (Barbour, 2005), given that all focus group participants were from the same career and university. The focus groups were carried out with undergraduate students (average 22-year-old) of Physical Chemistry I course of the fifth semester at the BA in Chemical Education and Chemistry Pedagogy during the academic year 2017 and 2018.



**Scheme 1.** Components into the design of Module: Requirement of the World Health Organization on Chagas disease, for training of Pre-service Chemistry Teachers.

## DISCUSSION

This research shows evidence that students' perceived the use of software of computational chemistry as effective tool to aid in the learning of chemistry concepts and development of scientific skills. Moreover, these tools were positively valued by the students in the context of training of pre-service chemistry teacher. The students reflect on the use of their acquired TSK in a potential pedagogical context. This finding could be indicating that pre-service chemical teachers should first acquire TSK and then develop their TPASK in a pedagogical context using a RWP in science for teaching chemistry with emerging technologies.

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