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Grande Área: Ciências Exatas e da Terra e Engenharias

PROFICIÊNCIA EM LEITURA EM LÍNGUA INGLESA

Adapted from: **Taking the experiment to cyberspace – Kungl. Vetenskaps Akademien:** The Royal Swedish Academy of Sciences.
Source:https://www.nobelprize.org/nobel_prizes/chemistry/laureates/2013/popular chemistryprize2013.pdf

[1] Chemical reactions occur at lightning speed; electrons jump between atoms hidden from the prying eyes of scientists. The Nobel Laureates in Chemistry 2013 have made it possible to map the mysterious ways of chemistry by using computers. Detailed knowledge of chemical processes makes it possible to optimize catalysts, drugs and solar cells. Chemists all over the world devise and carry out experiments on their computers on a daily basis. With the help of the methods that Martin Karplus, Michael Levitt and Arieh Warshel began to develop in the 1970s, they examined every tiny little step in complex chemical processes that are invisible to the naked eye.

[2] In order for you, the reader, to get an idea of how mankind can benefit from this, we begin with an example. Put your lab coat on, because we have a challenge for you: to create artificial photosynthesis. The chemical reaction occurring in green leaves fills the atmosphere with oxygen and is one prerequisite for life on Earth. But it is also interesting from an environmental perspective, because If you can mimic the photosynthesis you will be able create more efficient solar cells. When water molecules are split oxygen is created, but also hydrogen that could be used to power our vehicles. So there is ample reason for you to get engaged in this project. If you succeed, you could contribute to solving the problem with greenhouse effect.

[3] A picture says more than a thousand words — but not everything. As a first step you will probably go online and find a three dimensional image of the proteins that govern the photosynthesis. Such images are freely accessible in large databases on the internet. In your computer you can twist and turn the image as you like. It unveils gigantic protein molecules consisting of tens of thousands of atoms. Somewhere in the middle, there is a little region called the reaction center. This is where the water molecules are split. However, only a few atoms are directly involved in the reaction. Among other things, you see four manganese ions, one calcium ion and several oxygen atoms. The image clearly shows how atoms and ions are positioned in relation to each other, but it says nothing about what these atoms and ions do. This is what you need to find out. Somehow, electrons must be extracted from the water and four protons need to be taken care of. How does that happen? The details of this process are virtually impossible to map using traditional methods of chemistry. Many things happen in a fraction of a millisecond — a rate that rules out most kinds of test tube experiments. From the image that you have in your computer, it is also difficult to guess the reaction process, because it was taken when the proteins were in a state of rest. When sunlight hits the green leaves, however, the proteins are filled with energy and the entire atomic structure is changed. In order to understand the chemical reaction you need to know what this energy-filled state looks like. This is where you summon the help of the computer programs that the Nobel Laureates in Chemistry 2013 have laid the foundation for.

[4] Combining the best of both worlds. Previously when scientists wanted to simulate molecules on computers, they had software at their disposal that was based upon either classical Newtonian physical theories or quantum physics. Both had their strengths and weaknesses. The classical programs could calculate and process large chemical molecules. They would only display molecules in a state of rest, but gave chemists a good representation of how the atoms were positioned in the molecules. However, you could not use these programs to simulate chemical reactions. During the reaction, the molecules are filled with energy; they become excited. Classical physics simply have no understanding for such states, and that is a severe limitation. When scientists wanted to simulate chemical reactions, they had to turn to quantum physics; the dualistic theory where electrons can be both particles and waves simultaneously and where Schrödinger's famous cat, hidden in its box, can be both alive and dead. The strength of quantum physics is that it is unbiased and the model will not include any of the scientist's preconceptions.

[5] Therefore such simulations are more realistic. The downside is that these calculations require enormous computing power. The computer has to process every single electron and every atomic nucleus in the molecule. This can be compared to the number of pixels in a digital image. Many pixels will give you a high resolution, but also require more computer resources. Similarly, quantum physical calculations yield detailed descriptions of chemical processes, but require powerful computers.

RESPONDA DE ACORDO COM O TEXTO. AS RESPOSTAS DEVEM SER EM PORTUGUÊS

1) De acordo com o Parágrafo [1], os cientistas contemplados com Prêmio Nobel de Química de 2013 conseguiram um grande feito científico, a descoberta de um mistério. (3,0 pontos / 1,5 ponto cada).

a) Explique o que este feito tornou possível.

Resposta esperada: (elaborações contendo este conteúdo)

Tornou possível mapear os caminhos da química usando computadores, o que possibilita otimizar catalisadores, drogas e células solares.

b) Qual grande vantagem trouxe para a Química e para os cientistas do mundo?

Resposta esperada: (elaborações contendo este conteúdo)

A grande vantagem para os cientistas é que agora podem idealizar e executar experimentos químicos em seus computadores no dia a dia.

2) De acordo com o Parágrafo [2], o autor propõe um desafio ao leitor. (3,0 pontos / 1,5 ponto cada).

a) Qual é o desafio?

Resposta esperada: Criar fotossíntese artificial

b) Qual a relevância desta experiência na perspectiva do meio ambiente e da poluição causada pelos automóveis?

Resposta esperada: Como é possível imitar a fotossíntese, poderíamos criar células solares mais eficientes. Seria possível criar hidrogênio para abastecer os carros a partir de moléculas de agua que fossem desmembradas.

3) Nos Parágrafos [3 e 4], o texto fala sobre a importância das imagens tridimensionais para a compreensão das estruturas moleculares das proteínas, mas apresenta também uma limitação dos programas de computação. Explique essa limitação. (1,0 ponto)

Resposta esperada: Os programas de computação não podem similar reações químicas, dado que as moléculas estão cheias de energia e tornam-se agitadas. A limitação deve-se ao fato da física quântica não compreender esses estados.

4) Assinale **(V)** para as alternativas verdadeiras e **(F)** para as falsas: (2,0 pontos)

FALSO	Martin Karplus, Michael Levitt e Arieh Warshel começaram a desenvolver métodos que os auxiliavam a examinar detalhadamente os processos químicos visíveis à olho nu. **[P1]**
VERDADEIRO	A imagem das moléculas mostra como se posicionam os átomos em relação uns aos outros, mas não as suas funções. **[P3]**
VERDADEIRO	A teoria dualística da física quântica era utilizada quando os cientistas desejavam simular reações químicas. **[P4]**
FALSO	A vantagem da física quântica sobre a química por imagens computadorizadas é a utilização de equipamentos menos potentes. **[P5]**

5) Qual das opções abaixo melhor traduz o trecho transcrito a seguir: (1,0 ponto)

The strength of quantum physics is that it is unbiased and the model will not include any of the scientist's preconceptions.

	A vantagem da física quântica é que ela não se baseia em modelos previamente testados
	A força da física quântica é o seu modelo de base que não inclui preconceitos dos cientistas
X	A física quântica tem a vantagem de ser neutra e seu modelo desconsiderar qualquer concepção prévia dos cientistas.