Predictive electrochemistry: will it be possible?

M. A. Páez¹

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Establishing the standard potential of charge transfer of complex half-reactions is not trivial. Regarding this, let us try to analyze what happens when we have a surface that contains several metallic components. And this surface possesses a microstructure resulting from a heat treatment process, which were dosed according to a temperature–time transformation diagram. The result is not just a set of different metals co-existing on the surface. The result is, in general, a solid solution or a phase mixture composed of different elements, decorated by microstructures of two or more elements, known as second phases and whose presence is attributed to the variation in solubility with the temperature of each element in the mixture during solidification.

It is clear that a magnified and instantaneous realistic vision of a system like the one described, when altered with a potential difference in an ionic medium, would reveal a distribution of redox potentials at a given moment. However, it is not easy to determine which would be the constituents of the half-reactions associated to each Ox/Red pair from which originate the global potential difference. In general, these metals are not noble, so their stability as a metal in the presence of an ionic medium and even, in the presence of oxygen at high relative humidities, is absolutely limited, and the redox pairs could correspond to $MxOy/M^{+n}$ species type o, a combination of oxidized species $MxOy/MxOHy/M^{+n}$. So, the first step apparently would be to modify the components of the semi-reactions. What would be the tools to consider? Chemical affinity determinations? According to what parameter or property should we define them? Will it be possible to set Debye Hückel type models on an electrode interface? The challenge for Debye Hückel was to determine the average ionic activity coefficient that corrected the activity coefficients that explain

the interactions, when these are very intense, such as those of the Coulombic type, and with them to correct the chemical potential in solutions that contain species load (ions). Is it possible to theoretically define a parameter that, calculated from basic principles, corrects the standard potential of redox systems (Ox/Red)? It certainly is a challenge. Today, we have (i) some databases associated with important parameters of chemistry and physics in electrochemistry; (ii) advanced theoretical chemistry, the contribution of which has been important in explaining the behavior of the electrodes or the probabilities of interaction at the electrode interfaces; (iii) advanced theoretical physics, particularly in interface models; and very importantly (iv) the engineering sciences associated with materials.

How powerful the theoretical development would be for predictive electrochemistry of complex interfaces, both in chemical composition and in physical properties. This should be the result of removing the barriers between theoretical chemists, theoretical physicists, theoretical engineers, and, very importantly, theoretical mathematicians, who help establish by means of effective algorithms the superposition of the different factors influencing the redox property. The above is absolutely relevant today. Everything indicates a substantial progress in the development of new and advanced materials, for applications in strategic areas like energy, the environment, air and land transport, aerospace development, biomedicine, etc. This is undoubtedly the task of tomorrow, combining knowledge and efforts to develop predictive electrochemistry of interfaces/interphases in complex systems.

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✉ M. A. Páez
maritza.paez@usach.cl

¹ Departamento de Química de los Materiales, Facultad de Química y Biología, Universidad de Santiago de Chile, Av Libertador B.O'Higgins, 3363 Santiago, Chile