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Sommario/riassunto	"Electrochemistry and electrocatalysis are at the forefront of many technological fields related to solving the grand challenges encountered in advanced energy solutions, personalized medicine, and environmental issues. Electrochemical technologies of interest include, among others, batteries, CO2 mitigation, various sensor technologies, water purification, molecular electronics, fuel-cells, hydrogen powered energies, and solar-powered renewable technologies. To improve upon existing electrochemical technologies in a rational way, understanding and controlling the atomic scale properties of the electrochemical interface is vital. In particular, the connection between atomic scale surface chemistry and the electrocatalytical performance needs to be established. Rational design of better electrocatalysts working in complex electrochemical environments needs insight from experiments, computational methods, as well as theoretical approaches. While experimental electrochemical and spectroelectrochemical methods are well-established and can often be routinely applied, theoretical and computational methods have not yet reached the same level of maturity. The lack of generally accepted and applicable computational and theoretical tools is due to the high

complexity of the electrochemical interface which provides a number of challenges for atomic scale theory and modelling. Specific challenges include; (i) inclusion of the electrode potential, (ii) the need for several time and length scales to assess both thermodynamic and kinetic properties of the solid-liquid interface, and (iii) a quantum mechanical treatment to describe chemical bond making and breaking"--