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Preface
Jean-Louis Rivail Honorary Issue

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Professor Jean-Louis Rivail

This issue contains a selection of papers presented at the meeting "Modeling Chemical Reactivity: From Gas-Phase to Solution and Enzymes" held at Nancy, France, 16-18 July 2003.[1] It was organized in honor of Professor Jean-Louis Rivail on the occasion of his official University retirement.

Professor Rivail was born in La Mure (Isère, France) in 1937. He moved to Nancy in 1957 where he obtained the degree of Engineer in Chemistry at the ENSIC in 1960 and the PhD in 1964 working under the supervision of Professor Jean Barriol. After a post-doctoral stay at Oxford, where he worked with Prof. Coulson, he came back to Barriol's Theoretical Chemistry group at the University of Nancy and obtained an Assistant Professor position in 1965. Quickly, he advanced to a Full Professor position (1970) and, after the retirement of Professor Barriol in 1975, became the director of the Theoretical Chemistry group.

One of his most remarkable innovations in the French teaching system was the creation in 1984 of a national master diploma (DEA) on Computational and Theoretical Chemistry that offers students a thorough training in both computer sciences and theoretical chemistry. After obtaining the DEA, most students additionally pursue a PhD thesis and post-doctoral training. Former students of Jean-Louis Rivail are now working in chemical and pharmaceutical companies (L'Oreal, Michelin, Aventis,...) or occupy different positions in academia, the CNRS, or the INSERM.

Jean-Louis Rivail has also played an important role in the French research administration. Among other responsibilities, he has been a member of the CNRS National Committee and the President of the Physical Chemistry division of the French Chemical Society. He is also the President of the Scientific Council of the CINES, which is the CNRS computer center at Montpellier.

Professor Rivail is the European Editor of *Theochem* and has been (or in some cases continues to be) a member of the editorial board of other journals such as *Chemical Physics Letters*, the *Journal of Molecular Modeling*, and the *Journal of Physical Organic Chemistry*. He has organized many national and international meetings, including the First European Conference on Computational Chemistry in 1994 and the Xth International Congress of Quantum Chemistry in 2000. Recent honors he has received include the Süe Award of the French Chemical Society and the Catalán-Sabatier Award of the Spanish Royal Chemical Society. He is also an associated member of the Stanilas Academy.

As a researcher, the career of Jean-Louis Rivail has been particularly fruitful. His work has been characterized by a persistent effort to develop physical models and computational methods allowing the study of systems interacting with complex surroundings. His name is intimately associated with quantum mechanical continuum solvent models and with the theoretical study of solvated systems, an area that he began to develop in the early 1970s. At that time, quantum chemistry was essentially limited to the study of isolated systems but Jean-Louis Rivail's work opened a key new avenue of research that greatly contributed to reducing the gap between theory and experiment. Nowadays, applications of continuum models have become routine and several implementations are available. However, the two seminal papers published in 1973 and 1976—by Jean-Louis

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Rivail in collaboration with Daniel Rinaldi—established the basic fundamentals of the approach. More recently, Jean-Louis Rivail has contributed to the growing popularity of the combined quantum mechanics and molecular mechanics (QM/MM) techniques by developing a formalism for describing QM/MM frontier bonds. This approach is extremely useful for investigating very large systems like those encountered in biochemical processes. Indeeed, enzymatic catalysis represents one the most modern and appealing fields of application.

Today, Jean-Louis Rivail is an Emeritus Professor at the Henri Poincaré University. Contributions to this special issue are dedicated to him as a tribute in recognition of the important role he has played (and continues to play) in the field of theoretical and computational chemistry over the last several decades.

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