

Preface

The molecular state of matter is characterized by relatively rigid structures, by recurrent asymmetries, by strong covalent bonding, and by discrete energy levels. Continuous conductive materials such as metals or small gap semiconductors are generally periodic, delocalized structures with continuous energy level bands. When these materials are mixed, it is challenging to obtain an appropriate theoretical description, but it is equally rewarding to investigate the behaviors that may attain. Molecular electronics deals with precisely these issues, and how they are manifested in the transport, excitation, structural and frequency response of these hybrid continuum/discrete structures.

Molecular electronics really began with the pioneering work by Mann and Kuhn [J. Appl. Phys. 42 (1971) 4398] on transport through surface adlayers. It was greatly advanced by the development of scanning probe microscopy that could both make measurements and do assembly at the individual molecule or few-molecule level, and by the development of self-assembly methodologies to create such extensive structures. The field has progressed very rapidly, as evidenced by the decision of the editors of Science Magazine that “molecules get wired” was the outstanding scientific breakthrough in the year 2001.

The current Special Issue of Chemical Physics is therefore highly appropriate in its timing, and in its breadth of synthesis, measurement and model. The authors have combined to produce a remarkable set of papers that deal with how molecular junctions can be constructed and characterized, how molecular currents can be controlled and measured, how we can understand transport in molecular wire junctions, and more general thematic areas of molecular electronic behaviour.

The editors are grateful to Professor Ludwig Hofacker for encouraging this Special Issue, and to the authors for their timely submissions, and to the referees for their incisive remarks. We, guest editors, share the confident belief that this volume number on “Transport in Molecular Wires” captures an appropriate snapshot of this dynamic research area termed *molecular electronics* (at least within the limitations of finite space and time) in 2001/2002. Moreover, we hope that many readers will be invigorated in pursuing future own research by the contributions selected herein.

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