STRUCTURE AND DYNAMICS OF ATOMS AND MOLECULES: CONCEPTUAL TRENDS

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Structure and Dynamics of Atoms and Molecules: Conceptual Trends

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FOREWORD

The rivers run into the sea, yet the sea is not full

Ecclesiastes

What is quantum chemistry? The straightforward answer is that it is what quantum chemists do. But it must be admitted, that in contrast to physicists and chemists, "quantum chemists" seem to be a rather ill-defined category of scientists. Quantum chemists are more or less physicists (basically theoreticians), more or less chemists, and by and large, computationists. But first and foremost, we, quantum chemists, are conscious beings.

We may safely guess that quantum chemistry was one of the first areas in the natural sciences to lie on the boundaries of many disciplines. We may certainly claim that quantum chemists were the first to use computers for really large scale calculations. The scope of the problems which quantum chemistry wishes to answer and which, by its unique nature, only quantum chemistry can answer is growing daily. Retrospectively we may guess that many of those problems meet a daily need, or are say, technical in some sense. The rest are fundamental or conceptual. The daily life of most quantum chemists is usually filled with grasping the more or less technical problems. But it is at least as important to devote some time to the other kind of problems whose solution will open up new perspectives for both quantum chemistry itself and for the natural sciences in general.

When chemistry developed in the nineteenth century, its explanatory systems began to separate from those of physics, as peculiarly chemical theories of molecular structure and of reactivity were conceived. By the early twentieth century attempts were made to heal this rift and perhaps the most influential of these was the creation of the electronic theory of valency.

However it was not until the development of quantum mechanics in the late nineteen- twenties that it became clear how a proper reconciliation should be effected. It is in this context that quantum chemistry rises as a subject of its own and

gets a very special place among the natural sciences. Quantum chemistry provides the conceptual apparatus by means of which chemical explanation is tied to the explanatory scheme of quantum mechanics, one of the most fundamental of all physical theories.

Until the nineteen-fifties - even though important numerical work was certainly carried out also before that time - the chief contribution of quantum chemistry to chemistry was in terms of concepts like atomic and molecular orbitals, resonance, hybridisation and many others. Since about nineteen- sixty the development of computers has led to a change in emphasis. The conceptual apparatus has remained largely that of previous generations but thanks to large scale sophisticated quantum chemical computations, quantitatively accurate results have made it possible to assist in an effective way the understanding of many phenomena in chemistry, physics, and biology. There can be no doubt about the tremendous quantitative successes that quantum chemistry has had in the last three decades. However, it may not be out of place to have a look retrospectively at different angles and to ask: Whether time might not be ripe for making a paradigm shift in the nature of the concepts that are used, for breaching the decorum to say what has not yet been said before because it has seemed too trivial to bother with or too embarrassing to own up to, and for showing us something that had been there all the time that we had not seen for ourselves.

That was our idea to launch "Conceptual Trends in Quantum Chemistry". This former collection of essays of a number of active quantum chemists has been appeared under the identical title in the early 1994. The present one has the same underlying idea, although it is slightly more specified by the purpose. We hope that both these

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