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Preface

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Enrico Clementi was our mentor, our colleague, and our good friend. He had an important impact on the scientific directions of the research of us and of many of our colleagues. The papers in this special issue reflect the broad and diverse research efforts that Enrico inspired and that his own research stimulated. His career spanned more than 50 years and he interacted with and influenced a wide range of people from students to peers to other senior members of the community active in research on the properties and electronic structure of matter.

Much of his career was at IBM. From the early 60's to 1974, he was at the IBM Research Laboratories in San Jose, California and from 1979 to 1991 he was at IBM in Poughkeepsie and Kingston. At IBM San Jose, he organized and managed Department K07, the department for Large-Scale Scientific Calculations, LSCC. The department reflected his vision that theory and computation could and should address a complete range of scientific studies. One group within Depart K07 was concerned with the accurate theoretical prediction of the properties of atoms and molecules; this Quantum Chemistry research project was also very close to Enrico's personal research interests. Other research areas in department K07 concerned the properties of condensed matter and the molecular dynamics of these systems. Finally, there was a group in K07 concerned with hydrodynamics and fluid flow. The efforts in K07 were intended to push the limits of computation to new extremes. This was done by developing new and powerful program systems and by having access to the most powerful computers of the time. Enrico's personal contribution to this program development was the IBMOL program system which could be used to carry our Hartree–Fock calculations on very large systems. For his calculations on the components of DNA, Enrico had to use the computers at IBM Yorktown, in New York, that were even more powerful than those at IBM San Jose to calculate the integrals needed to compute the wavefunctions for his research on DNA. These integrals were stored on several tapes and Enrico wanted to be certain that they would not be lost of damaged on the flight back to California from New York. To ensure their safety, he purchased two seats on his flight to California, he used one seat and the tapes 'sat' in the other seat. Enrico also guided the Quantum Chemistry project to develop the ALCHEMY program system which could carry out calculations of the electronic structure of small to modest size molecules to a level of accuracy, including electron correlation effects, to a level that was unprecedented at that time.

Enrico understood that progress in the development and application of large scale computations would be enhanced by having an active visitor program under which people would come for stays at IBM of order a year to collaborate with and contribute to the program development. For this, Enrico pioneered the IBM World Trade post-doctoral program to support visitors to IBM San Jose. The visitors to Department K07 would take away the knowledge and the skills that they learned as well as the programs they had helped to develop to their home institutions. In this way Enrico was instrumental in helping to spread the culture of scientific computation. This also made it possible for the visitors and for the IBMers in K07 to form personal friendships which, in many cases, lasted well after the time the visitors were at IBM. Much of this happened during the period when programs

were freely exchanged before the view that programs could be licensed or sold as a source of revenue. Once this happened, it became more difficult to exchange programs.

He stepped down from managing K07 to focus on his personal research once he became an IBM Fellow for his work on the development of scientific computation. Indeed, his interest in extending and broadening his research efforts lead him to leave IBM in 1974 to return to Italy, his native country. There he joined Montedison in Novara where he once again managed a group now more specialized in computational Chemistry. However, his vision of integrating computation from the atomistic to the macroscopic realms, lead him to rejoin IBM in 1979 and to form new groups at IBM in Poughkeepsie and Kingston. It was in this period that he organized and edited the MOTECC, Modern Techniques in Computational Chemistry, series of volumes that contained chapters describing different theoretical programs for computational chemistry. MOTECC-89 contains 15 chapters in over 600 pages while MOTECC-91 contains 33 chapters in over 1200 pages. The guest editors of this special issue all have been co-authors of chapters in these volumes. It is even more important that many of the leading groups in computational chemistry have contributed chapters to the MOTECC volumes. Enrico's passion for theoretical chemistry and, in particular Quantum Chemistry, lead him to move on from IBM to the University of Strasbourg in 1991.

At Strasbourg, he continued to make computation broadly available through the MECTECC series of volumes modeled after the MOTECC series of books but containing new contributions on new topics. For both the MOTECC and MECTECC volumes, the importance of parallel processing was stressed since this is a way to increase the power of computational chemistry by orders of magnitude. Enrico knew from his life's work that as we can increase computational power we can expand the solutions that theory can offer us. Although Enrico officially retired from Strasbourg in 2000 and returned to Italy to live in Como, he continued to work with his wife, Gina Corongiu, and to publish regularly. It was in this period that he worked on integrating and combining molecular orbital theory and valence bond theory in order to have the advantages of both of these theoretical approaches. In a sense, he was able to resolve the competition between Mulliken, a strong proponent of molecular orbital theory, and Pauling, an equally strong proponent of valence bond theory.

Enrico's received many honors and awards in his career. These included: Awarded an IBM Fellowship in 1968; the Teresiana Gold Medal of the University of Pavia; Fellow of the American Physical Society; Distinguished Research Professor at the Rensselaer Polytechnic Institute, Troy, New York; The Dirac Medal from WATOC awarded in 1987; the Boys Medal of the Royal Society awarded in 1996; Dr Honoris Causa of the University of Namur in 1999; President of the International Society for Quantum Biology in 2001; The Alexander von Humboldt Prize in 2001; The Dr Honoris Causa of the University of Oviedo in 2017; Enrico was elected a member of the International Academy of Quantum Molecular Science in 1994.

The papers in this special issue reflect the interests and the stimulation that the authors received from Enrico. The authors are from many different countries including the United States, and countries in Europe, and Asia. The topics range from small molecules to complex perovskite compounds; they include papers that deal with core-level processes and papers that are concerned with drugs to combat COVID infections. The electronic structure methods use both density functional theory and wavefunction theory. Depending on the scientific problems addressed, the methods are based on non-relativistic quantum mechanics or take into account relativistic effects. While most papers deal with bound electronic states,

continuum electrons are also described. Enrico would have appreciated the scope of the papers in this issue.

As well as his contributions to science, Enrico was avid to paint and some of us have been fortunate to see his paintings. He was a good friend to many and we enjoyed being with him as well as working with him. We are sad that Enrico passed away on 30 March 2021. We have missed being in his company and spending time with him both for science and for pleasure. It is our hope that this issue will be a tribute to his many contributions and that the papers in the issue will honor his memory.

Data availability statement

No new data were created or analysed in this study.

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