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Sommario/riassunto	The QM/MM method, short for quantum mechanical/molecular mechanical, is a highly versatile approach for the study of chemical phenomena, combining the accuracy of quantum chemistry to describe the region of interest with the efficiency of molecular mechanical potentials to represent the remaining part of the system. Originally conceived in the 1970s by the influential work of the the Nobel laureates Martin Karplus, Michael Levitt and Arieh Warshel, QM/MM techniques have evolved into one of the most accurate and general approaches to investigate the properties of chemical systems via computational methods. Whereas the first applications have been focused on studies of organic and biomolecular systems, a large variety of QM/MM implementations have been developed over the last decades, extending the range of applicability to address research questions relevant for both solution and solid-state chemistry as well. Despite approaching their 50th anniversary in 2022, the formulation of improved QM/MM methods is still an active field of research, with the aim to (i) extend the applicability to address an even broader range of research questions in chemistry and related disciplines, and (ii) further push the accuracy achieved in the QM/MM description beyond that of established formulations. While being a highly successful approach on its own, the combination of the QM/MM strategy with other established theoretical techniques greatly extends the capabilities of the

computational approaches. For instance the integration of a suitable QM/MM technique into the highly successful Monte-Carlo and molecular dynamics simulation protocols enables the description of the chemical systems on the basis of an ensemble that is in part constructed on a quantum-mechanical basis. This eBook presents the contributions of a recent Research Topic published in Frontiers in Chemistry, that highlight novel approaches as well as advanced applications of QM/MM method to a broad variety of targets. In total 2 review articles and 10 original research contributions from 48 authors are presented, covering 12 different countries on four continents. The range of research questions addressed by the individual contributions provide a lucid overview on the versatility of the QM/MM method, and demonstrate the general applicability and accuracy that can be achieved for different problems in chemical sciences. Together with the development of improved algorithms to enhance the capabilities of quantum chemical methods and the continuous advancement in the capacities of computational resources, it can be expected that the impact of QM/MM methods in chemical sciences will be further increased already in the near future.