Communications in Computational Chemistry
Commun. Comput. Chem. Vol. 8, No. 1, 97–125
doi: 10.4208/cicc.2026.21.01

Review

Molecular Quantum Dynamics: Recent Perspectives

Fabien Gatti[1,*]

[1] *Université Bourgogne Europe, CNRS, Laboratoire Interdisciplinaire Carnot de Bourgogne ICB UMR 6303, F-21000 Dijon, France.*

[*] Corresponding author: fabien.gatti@u-bourgogne.fr.

Received 22 Jan. 2026; Accepted (in revised version) 4 Mar. 2026

Abstract: This review aims to address the current state of the art in the field of Molecular Quantum Dynamics (MQD), where the Schrödinger equation, either in its time-independent or time-dependent form, is solved for the nuclei involved in molecular processes. This is not an exhaustive review of the field, which is far too broad for such an undertaking. Instead, we focus primarily on methods that have enabled the study of larger systems, the size of molecular systems has long been a persistent limitation in the field. We also offer some perspectives, showing that, under certain conditions, it is now becoming possible to treat larger systems(as defined within the scope of this field) in a more systematic way. These advances suggest that MQD's full potential remains to be fully explored.

Key words: molecular quantum dynamics, molecules, quantum, theory.

1. Introduction

This review focuses on the field of Molecular Quantum Dynamics (MQD) [1-5], in which both the electrons and nuclei of a molecular system are treated using a fully quantum-mechanical framework. More specifically, we concentrate on methods in which the Schrödinger equation, in either its time, dependent or time-independent form—is solved for the nuclear degrees of freedom. We do not address semi-classical [6-10] or mixed classical-quantum approaches in this context. With even stronger reason, we do not deal with molecular dynamics (MD) methods, despite their great importance in theoretical chemistry, where the nuclei are treated classically. In particular, despite similarities in terminology, the field of "Molecular Quantum Dynamics" must be clearly distinguished from what is sometimes called "Quantum Molecular Dynamics. In the latter case, the word "quantum" refers to the quantum treatment of the electrons, but, unlike in MQD, the nuclei are treated classically.

The significance of quantum effects in chemistry—such as tunneling, quantum resonances, and quantum interference—is now well established and theoretical chemistry has recently undergone a significant paradigm shift, driven by the more systematic inclusion of quantum nuclear effects in molecular dynamics. Although methods to account for these effects—whether exactly or approximately—were first developed as early as the late 1960s, their critical importance has never been as clearly recognized by the theoretical chemistry community as it is today. This is exemplified by the recent extension of path integral molecular dynamics [11-13] to go beyond the classical treatment of nuclear motion in condensed matter systems [14-16]. For instance, an accurate description of proton transfer mechanisms requires the inclusion of both proton tunneling and the zero-point energy of the molecular system [17]. Similarly, the increasingly acknowledged role of quantum coherence in non-Born–Oppenheimer processes in photochemistry [18,19] has motivated sustained efforts to move beyond traditional approaches such as Ehrenfest dynamics, trajectory surface hopping and more elaborate methods developed by J. Liu and coworkers [20-22], where nuclei are treated (semi)-classically. In practice, however, simulations of nuclear quantum effects remain intrinsically approximate.

Beyond the need for reference methods to assess the validity of more approximate techniques, a fully variational approach that solves the Schrödinger equation is indispensable for a comprehensive description of the emergent quantum phenomena in molecular systems. Molecules are the fundamental building blocks of everyday life. A comprehensive understanding of Molecular Quantum Dynamics (MQD)—and the ability to control it—holds promise for transformative applications, particularly in chemistry, materials science, energy science, biology, and medicine. Such control could enable a fundamental shift from traditional trial-and-error approaches to rational and purposeful molecular design.

Conventional industrial chemical processes are typically governed by macroscopic external parameters, such as temperature, pressure, concentration, solvent choice, or the addition of catalysts. While these methods are effective, they often result in significant energy waste and the generation of large quantities of unwanted by-products. These shortcomings give rise to two major societal challenges: unsustainable energy consumption and environmental pollution. Addressing these issues requires studying chemical processes at their most fundamental level, where quantum effects govern behavior in the microscopic domain. Achieving such an understanding would enable unprecedented levels of control over chemical reactions. In this way, the chemistry of the future—and the innovative applications it enables—will be fundamentally quantum in nature.