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investigated the atomistic and dynamical mechanism of polaron formation in methylammonium lead iodide perovskite (MAPbI_3), which is a representative perovskite solar cell absorber, through the quantum mechanical

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Quantum dynamics simulations. The simulations were conducted on the spatial scale of several nanometres, which can describe charge localization and the associated structural deformation, using the divide-and-conquer-type density-functional

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method, which ...

Quantum
mechanical
molecular dynamics
simulations of ...

Molecular dynamics
simulation (MD
simulation) had a
great advantage in
dealing with large
molecular systems
such as ILs,

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especially without considering the electronic structure . Yan et al. [28] carried out MD simulation of the electronic polarization model of ILs, and the simulation results have a good correlation with the experimental results.

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calculation,
molecular dynamics
simulations~~

Molecular dynamics simulations were used to probe the mechanisms of viral assembly. The entire STMV particle consists of 60 identical copies of one protein that

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make up the viral capsid (coating), and a 1063 nucleotide single stranded RNA genome. One key finding is that the capsid is very unstable when there is no RNA inside.

~~Molecular dynamics~~
~~—Wikipedia~~

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decades, to support experimental observations and measurements, quantum mechanical molecular dynamics (QMMD) simulations with reasonable accuracy and efficiency have significantly unraveled structural,

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energetic, and
dynamical
properties of
excess proton in
aqueous
environments.

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dynamics ...~~

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millions of atoms at
a time but does not
capture quantum-
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interactions
between electrons.

Today chemists and
materials scientists
can run molecular
dynamics
simulations of
millions of atoms,
though without an

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explicit
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individual electrons.

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implemented a
quantum molecular
dynamics simulation
incorporating
nonadiabatic

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transitions on
massively parallel
computers to study
photoexcitation
dynamics of
electrons and ions.

The nonadiabatic
quantum molecular
dynamics (NAQMD)
simulation is based
on Casida ' s linear
response time-
dependent density

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Quantum theory to describe electronic excited states and Tully's fewest-switches surface hopping approach to describe nonadiabatic electron-ion dynamics.

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Simulations The
first step is to
optimise the
geometry to
remove any large
forces from the
starting
configuration. Large

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initial forces can
cause integration
problems in the
following molecular
dynamics
calculations.

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from molecular
dynamics
simulations ...~~

Molecular dynamics
and its relation to
other methods of

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Computer simulation

Computer simulations in condensed matter physics aim to calculate structure and dynamics from atomistic input [1 – 4]. The theoretical basis of this approach is statistical thermodynamics.

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(ETN) “ MOQS –
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Quantum simulation
of quantum
chemistry is one of
the most compelling
applications of
quantum computing.
It is of particular
importance in areas
ranging from

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materials science,
biochemistry, and...

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Simulations;
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polycrystalline

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paper, we explore
in detail the way in
which quantum
decoherence is
treated in different
mixed~~

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molecular dynamics~~

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algorithms. The
quantum
decoherence time
proves to be a key
ingredient in the
production of
accurate
nonadiabatic
dynamics from
computer
simulations. Based
on a short time
expansion to a
semiclassical

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golden rule
expression due to
Neria and Nitzan [J.
Chem. Phys. 99,
1109 (1993)], we
develop a new
computationally
efficient method for
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~~Quantum
decoherence and
the isotope effect in
condensed ...~~

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Since the first work of Fermi, Pasta, and Ulam in 1955, molecular dynamics (MD) simulation has frequently been used to investigate and predict the properties of condensed matter. For a crystal, these calculations are valid in the classical limit, i.e.,

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for temperatures higher than the Debye temperature. For example, in the case of a harmonic interatomic potential, the calculated heat capacity is constant at all temperatures and equals the limit value of Dulong and Petit (1819).

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bath for molecular
dynamics simulation~~

Abstract A
combined quantum
mechanical (QM)
and molecular
mechanical (MM)
potential has been
developed for the
study of reactions
in condensed
phases. For the

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quantum mechanical
calculations
semiempirical
methods of the
MNDO and AM1
type are used, while
the molecular
mechanics part is
treated with the
CHARMM force
field.

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quantum mechanical~~

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Here,
quantum – classical
molecular dynamics
(MD) and free
energy methods are
used to disclose the
two-metal-
dependent
mechanism of
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bond cleavage in
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initio MD reveals a conformational rearrangement of the Mg²⁺-bound RuvC active site, which entails the relocation of H983 to act as a general base.

Catalytic
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This project is focused on the methods which avoid exponential curse of quantum dynamics. The ambition of the project is to create quantum analog of classical molecular dynamics capable of solving the time-dependent

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