Fast and accurate simulation of nuclear quantum effects in ab-initio molecular dynamics by a generalized Langevin equation

Fact Sheet

Project Information

NQEAIMD

Grant agreement ID: 272402

Project closed

Start date
1 July 2012

End date
30 June 2014

Funded under
Specific programme "People" implementing the Seventh Framework Programme of the European Community for research, technological development and demonstration activities (2007 to 2013)

Total cost
€ 200 049,60

EU contribution
€ 200 049,60

Coordinated by
THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD
United Kingdom

This project is featured in...

Objective

"Computer simulations of matter at the atomic level provide insights complementary to experiments in a number of different physical, chemical and biological problems. The quantum nature of nuclei is usually disregarded, because of the computational burden inherent in an accurate treatment. However, these nuclear quantum effects have important, qualitative consequences, in particular when light atoms such as hydrogen are present. Moreover, inelastic neutron scattering techniques have been developed in the past years, which probe experimentally the quantum distribution of proton velocities, and would benefit from the availability of inexpensive modeling tools.
Here we propose the development of a new methodology for treating nuclear quantum effects, which reduces computational effort without sacrificing accuracy by combining in a unified formalism path integral molecular dynamics and the ""quantum thermostat"", based on correlated-noise stochastic equations.
We expect in this way to be able to treat routinely nuclear quantum effects together with an accurate, first-principles evaluation of inter-atomic forces, while so far this has only been attempted occasionally and with great computational effort.
These theoretical developments will be accompanied by applications to problems of fundamental and technological relevance. After having demonstrated the reliability of our approach on a few simple, controlled examples, we will tackle the problem of ab-initio water, in particular with reference to recent inelastic neutron scattering experiments performed at ISIS.
At a later stage we will choose a more complex problem to demonstrate our approach. Among the possible applications, hydrogen-storage materials are particularly promising, also considering the opportunity of a collaboration with the experimental group of Prof. Bill David, who has been performing leading-edge experiments on complex hydrides in the past few years at the Rutherford Appleton Laboratories in Oxfordshire."

Fields of science (EuroSciVoc)

Programme(s)

FP7-PEOPLE - Specific programme "People" implementing the Seventh Framework Programme of the European Community for research, technological development and demonstration activities (2007 to 2013)

Topic(s)

FP7-PEOPLE-2010-IEF - Marie-Curie Action: "Intra-European fellowships for career development"

Call for proposal

FP7-PEOPLE-2010-IEF
See other projects for this call

Funding Scheme

MC-IEF - Intra-European Fellowships (IEF)

Coordinator

THE CHANCELLOR, MASTERS AND SCHOLARS OF THE UNIVERSITY OF OXFORD

EU contribution

€ 200 049,60

Total cost

No data

Address

WELLINGTON SQUARE UNIVERSITY OFFICES
OX1 2JD Oxford
United Kingdom

Region

South East (England) > Berkshire, Buckinghamshire and Oxfordshire > Oxfordshire

Activity type

Higher or Secondary Education Establishments

Links

Contact the organisation Website
Participation in EU R&I programmes
HORIZON collaboration network

Last update: 2 August 2019

Permalink: https://cordis.europa.eu/project/id/272402