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

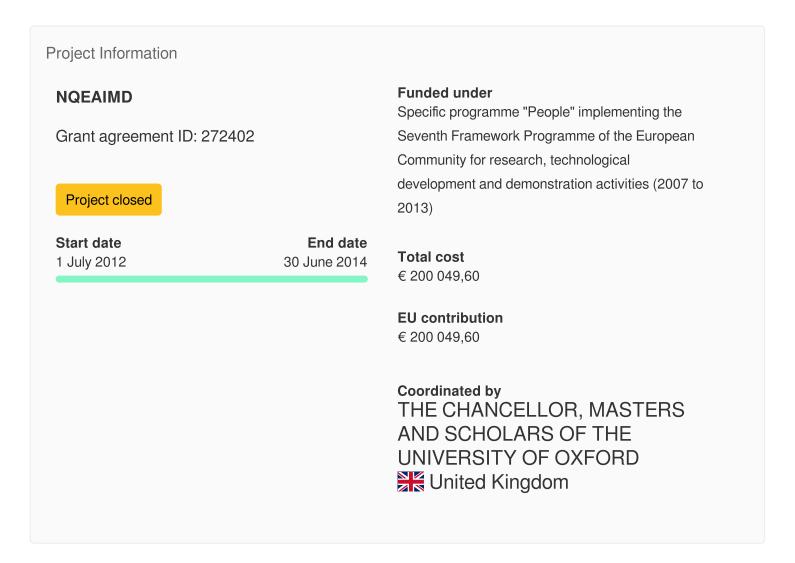


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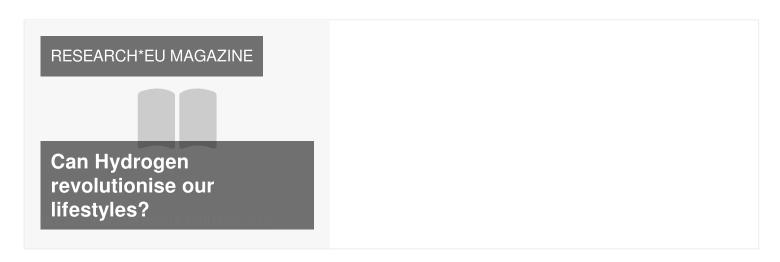


# Fast and accurate simulation of nuclear quantum effects in ab-initio molecular dynamics by a generalized Langevin equation

#### **Fact Sheet**



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# **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 abinitio 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."

## 



## 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

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Region

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

Activity type

#### **Higher or Secondary Education Establishments**

Links

Contact the organisation Website Medicipation in EU R&I programmes Medicipation in EUR Medicipation in EUR

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