

# Ab Initio Quantum Molecular Dynamics

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We discuss our recent progress in solving the electronic and nuclear Schrodinger equations simultaneously, emphasizing accurate modelling of tunnelling and nonadiabatic effects. The ab initio multiple spawning (AIMS) method developed for this purpose uses a Gaussian wavepacket expansion for the nuclear degrees of freedom and ab initio quantum chemical methods for the computation of potential energy surfaces and their nonadiabatic couplings. The accuracy of the dynamical and electronic structure methods used is assessed, and a few applications to photochemistry and proton transfer are presented.