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Molecular Dynamics of Large Systems with Quantum Corrections for Selected Nuclei[1] SOPHYA GARASHCHUK, University of South Carolina — The classical dynamics of nuclei is adequate in many situations, providing insight into chemical processes. Yet it is well-known that quantum features of nuclear behavior – the zero-point energy, tunneling and nonadiabatic dynamics – are sometimes important. We are interested in the regime when quantum-mechanical (QM) behavior of nuclei of a few selected bonds modestly affects reactivity while the full QM treatment is unfeasible due to exponential scaling of numerical cost with the system size for the conventional methods. To make qualitative predictions and cheap estimates of the nuclear QM effects we are developing approximate dynamics based on the quantum trajectory (QT) formulation of the Schrodinger equation. The QM effects are incorporated through the quantum potential, computed in the "mean-field" approximation, acting on the trajectory ensemble in addition to the classical potential. Large molecular systems are described in a mixed quantum/classical QT framework with the QM correction incorporated into selected degrees of freedom. The approach is applied to study adsorption of quantum hydrogen colliding with the graphene model, C37H15.

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