Abstract Submitted
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Stochastic Quantum Molecular Dynamics HEIKO APPEL, MASSIMILIANO DI VENTRA, University of California, San Diego — Conventional molecular dynamics (MD) approaches like Car-Parinello (CPMD), Born-Oppenheimer (BOMD) or Ehrenfest MD have in common that the electronic degrees of freedom are always described in terms of a closed quantum system. By construction, CPMD and BOMD only refer to the ground-state Born-Oppenheimer surface, whereas Ehrenfest MD can take into account electronic excitations. However, in all cases the description in terms of a closed electronic system excludes the possibility of electronic relaxation and decoherence. Based on stochastic Kohn-Sham equations, a new MD approach is presented that allows for an open quantum system description of both the electronic and the nuclear degrees of freedom. The new approach is illustrated with a MD study of vibrational and rotational relaxation in 4-(N,N-dimethylamino)benzonitrile (DMABN). Reference: cond-mat/09082411.

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