Classical Nuclear Motion in Quantum Transport CLAUDIO VER-
DOZZI, GIANLUCA STEFANUCCI, CARL-OLOF ALMBLADH, Solid State The-
ory, Lund University-Sweden — An *ab initio* quantum-classical mixed scheme for the
time evolution of electrode-device-electrode systems is introduced to study nuclear
dynamics in quantum transport. Two model systems are discussed to illustrate the
method. Our results provide the first example of current-induced molecular desorp-
tion as obtained from a full time-dependent approach, and suggest the use of AC
biases as a way to tailor electromigration.

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