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Exploiting unitary invariance in ab initio molecular dynamics: Applications to spectral decomposition and surface reactions[1] MARK TUCKERMAN, New York University — The methodology of ab initio molecular dynamics, wherein finite-temperature dynamical trajectories are generated using forces computed "on the fly" from electronic structure calculations, has benefited significantly from its combination with maximally localized electronic orbitals. The latter exploit the unitary invariance of the total energy to generate orbitals with maximum spatial locality. These orbitals resemble the classic textbook picture of molecular orbitals and, hence, are useful tools for analyzing electronic structure. In addition, maximally localized orbitals, expanded in localized basis sets, are a key component in linear scaling methods. In this talk, it will be shown how techniques from quantum field theory can be used to reformulate ab initio molecular dynamics in such a way that maximally localized orbitals are generated automatically and dynamically as the calculation proceeds. As an application of the technique, it will be shown how IR spectra can be decomposed to reveal particular structures in aqueous solutions. A second application will focus on the addition of organic molecules to the Si(100)-2x1 surface.

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