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Coupling of electrons to the electromagnetic field in a localized basis¹ ROLAND ALLEN, Texas A&M University — A simple formula is obtained for coupling electrons in a complex system to the electromagnetic field. It includes the effect of intra-atomic excitations and nuclear motion, and can be applied in, e.g., first-principles-based simulations of the coupled dynamics of electrons and nuclei in materials and molecules responding to ultrashort laser pulses. Some additional aspects of nonadiabatic dynamical simulations are also discussed, including the potential of “reduced Ehrenfest” simulations for treating problems where standard Ehrenfest simulations will fail.

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Prefer Oral Session
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