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Semiclassical electron-radiation-ion dynamics: past successes and future extensions[1] ROLAND ALLEN, MENG GAO, PETRA SAUER, Texas A&M University, YUSHENG DOU, Nicholls State University — Treatments of photochemical reactions that employ "potential energy surfaces" and are based on the Born-Oppenheimer approximation have various limitations: (i) They typically include only about 2 nuclear degrees of freedom which are postulated to be most important. (ii) They typically put electons into an assumed intial state rather than properly treating the excitation of the molecule. (iii) They typically do not include a proper treatment of the de-excitation of the molecule at avoided crossings near conical intersections. For this reason we have used the complementary technique of semiclassical electron-radiation-ion dynamics (SERID), in which the position operator for each nuclear coordinate is replaced by its expectation value in the Heisenberg equation of motion. One is thus averaging over the various terms in the Born-Oppenheimer expansion of the total wavefunction for nuclei and electrons. Here we review some results which demonstrate the ultity of SERID, and we also discuss how it can be extended to (1) include ionization and (2) treat the time evolution of particular terms in the Born-Oppenheimer expansion, so that its principal limitation is circumvented.

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