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Mixed quantum/semiclassical studies of condensed-phase dynamics and spectroscopy[1] JEFFREY A CINA, PHILIP A KOVAC, Department of Chemistry Biochemistry, Oregon Center for Optical, Molecular, and Quantum Science — We report on theoretical and computational studies of molecular-level chemical dynamics and their time-resolved spectroscopic signatures for small molecules embedded in low-temperature crystalline-host environments. Our calculations are based on a mixed quantum mechanical/semiclassical theory, referred to as the variational fixed vibrational basis/Gaussian bath theory (v-FVB/GB), in which certain optically addressed coordinates driven to large-amplitude motion by laser pulses are treated fully quantum mechanically and a larger number of others executing small-amplitude motion are treated semiclassically. Model systems under investigation incorporate a dihalogen molecule isolated in a symmetrical cluster of rare-gas atoms, with the outer layer of host atoms bound together in a harmonic net that preserves the initial equilibrium structure, but emulates an extended medium by preventing dynamical reconstruction and host-atom evaporation.

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