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Quantum Dynamics of Energy Transfer under Shock Conditions[1]

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Classical molecular dynamics (MD) simulations predict efficient energy transfer from translational to vibrational modes near shock fronts in molecular solids. The validity of the classical description of collisional energy transfer under shock conditions has not been tested for extended systems. In this research effort, quantum mechanical (QM) simulations are used to study energy transfer in a system consisting of three collinear diatomic molecules and a stationary wall. A fast-moving projectile diatom collides with its neighbor initiating a collision cascade. The multiplicity of collisions precludes *a priori* prediction of the detailed collision dynamics. The time dependence of the six-degrees-of-freedom wave function is determined using QM time-dependent wave packet methods. Intra- and inter-molecular interactions are described using nearest-neighbor potentials. Probabilities for vibrational excitation and bond rearrangement are predicted as a function of the collision energy of the projectile for differing interaction potentials and atomic masses.

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