A combined quantum and classical approach to predict the C_{60} and C_{60} collisional product distribution at the experimental time-scale

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Collisions between C_{60} and C_{60} have been studied experimentally since 1996. For collision energies beyond the barrier the fusion reaction cross section increases with collision energy to a maximum value at around 100 eV and then decreases at higher energies. Quantum mechanical and classical reactive molecular dynamics were performed for C_{60} + C_{60} collisions to understand the dynamics and the kinetics of the reaction at collision energies 20 – 200 eV. The fusion barrier calculated by the Density functional Tight Binding theory(DFTB), 60 eV, is in excellent agreement with the experimental results, while classical dynamics underestimated the fusion barrier by 40 eV. DFTB is far more computationally expensive than the classical force field calculations, and a method must be very cheap computationally to be suitable for long trajectory simulations. In order to include the quantum mechanical degrees of freedom and to overcome the fusion barrier problem, we have performed DFTB simulations for the first 5 ps to model the collisional phase and then AIREBO(Adaptive Intermolecular Reactive Empirical Bond Order) classical reaction dynamics for 12 ns to reduce the computational cost. Thus, a DFTB+AIREBO approach is used to predict the product distribution at the experimental timescale. A single exponential decay Arrhenius kinetics used to determine the product distribution, which allowed extrapolation to microsecond timescale. The product distribution range of DFTB+AIREBO simulations is agree with the experimental results after 0.5 μs, in fact no fused products observed after 160 μs.