

Read Me

Files named `passivated.zip`, and `clean.zip` are compressed tar files containing multiple CASTEP output files of the `seed.md` format. In each case, the “seed” of the individual filename indicates the initial location of the impinging F2 molecule (A-F) and its orientation (alpha, beta, or gamma). More detail on this may be found in the associated paper. The file named `c4x4_stitched.zip` contains the same kind of data, but for a single trajectory in which ejection of a single fluorine atom occurs. The `seed.md` format contains, in plain text, the positions (R), velocities (V), and forces (F) corresponding to atoms within the system at successive times (T) during the simulated motion. R, V, and F values are in atomic units, while T values are in femtoseconds.

Files named `clean_spin.zip` and `passivated_spin.zip` are compressed tar files containing multiple plain text files relating to the spin parameters obtained during simulations. Names of individual files correspond to the trajectory files described above. Each file contains three columns of data – the first simply recording the time-step (each time-step increments the simulation time by 0.5 fs), the second contains the integrated net spin, and the third the integrated spin modulus. Note that the sign of the second column is essentially arbitrary, and may be reversed if desired (as long as one reverses it for the whole column).