Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Reaction Dynamics Inside Superfluid Helium Nanodroplets. The Formation of the Ne_2 Molecule From Ne + Ne@(^{4}He)$_N$

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Table S1. Parameters defining the helium and neon Cartesian grids for the helium nanodroplet with N=500.[a,b]

$\langle v_0 \rangle$ (m/s)	hz_{Ne} (Å)	hz (Å)	hx=hy (Å)
120	0.114	0.3	0.4
210	0.114	0.3	0.4
300	0.114	0.3	0.4
500	0.114	0.3	0.4
800	0.089	0.2	0.4
1200	0.067	0.2	0.4

[a] The parameters h refer to the spatial separation of the grids.

[b] The limits of the helium grid for this nanodroplet (radius=20.0 Å) have been taken as $x_{min}=y_{min}$=-26.0 Å and z_{min}=-30.0 Å and $x_{max}=y_{max}$=25.6 Å and z_{max}=29.7 Å for $\langle v_0 \rangle$ below 750 m/s; and $x_{min}=y_{min}$=-26.0 Å and z_{min}=-28.6 Å and $x_{max}=y_{max}$=25.6 Å and z_{max}=28.4 Å. The limits of the Ne atoms grid correspond to r_{min}=1.5 Å and r_{max}=30.0 Å (120 and 300 m/s) or 32.0 Å (above 300 m/s).

Table S2. Final propagation times for the helium nanodroplet with N=500.

$<v_0>$ (m/s)	t_{final} (ps)
120	188.2
210	204.7
300	195.5
500	128.2
800	177.1
1200	105.5

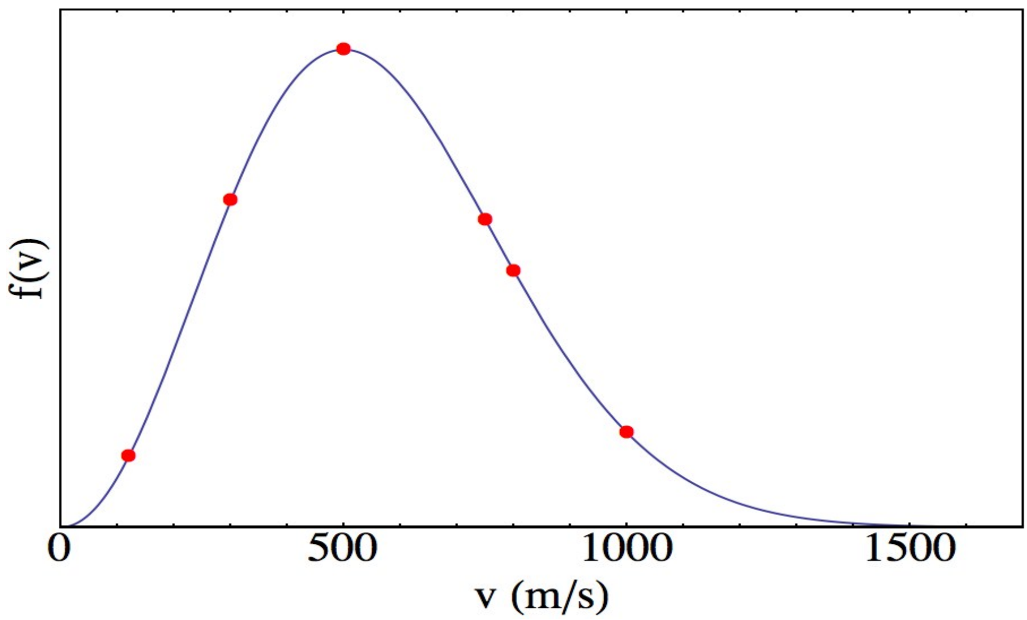

Figure S1. Maxwell velocity distribution of Ne in gas phase at a temperature of 300 K. The red points indicate the main selected velocities considered in this work.

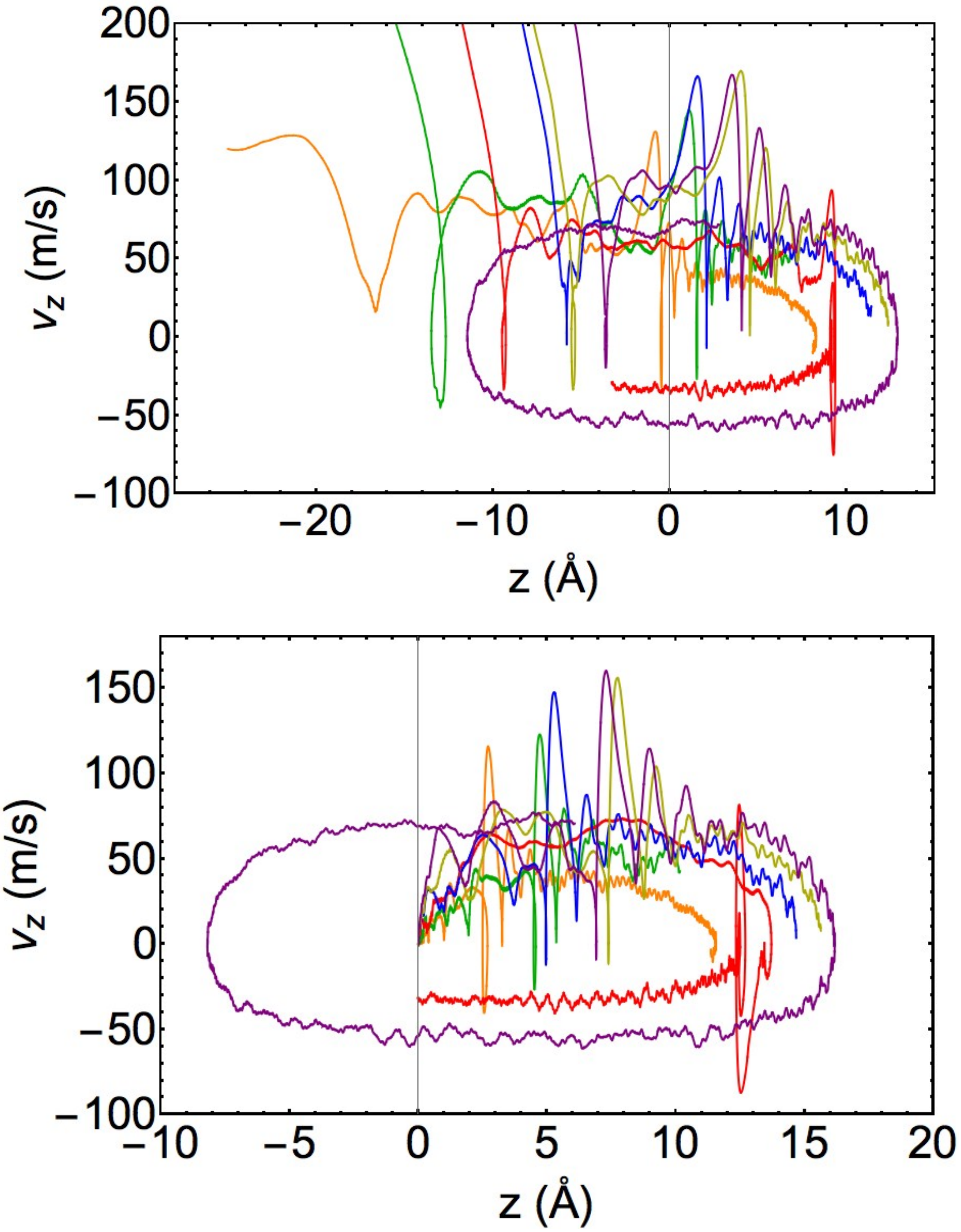

Figure S2. Trajectories of the mean values of the Ne atoms velocities and positions as a function of <v_0> (impinging Ne atom (up) and inner Ne atom (down)), for the nanodroplet with N=500: orange (120 m/s), green (300 m/s), red (500 m/s), blue (750 m/s), green olive (800 m/s) and violet (1000 m/s).

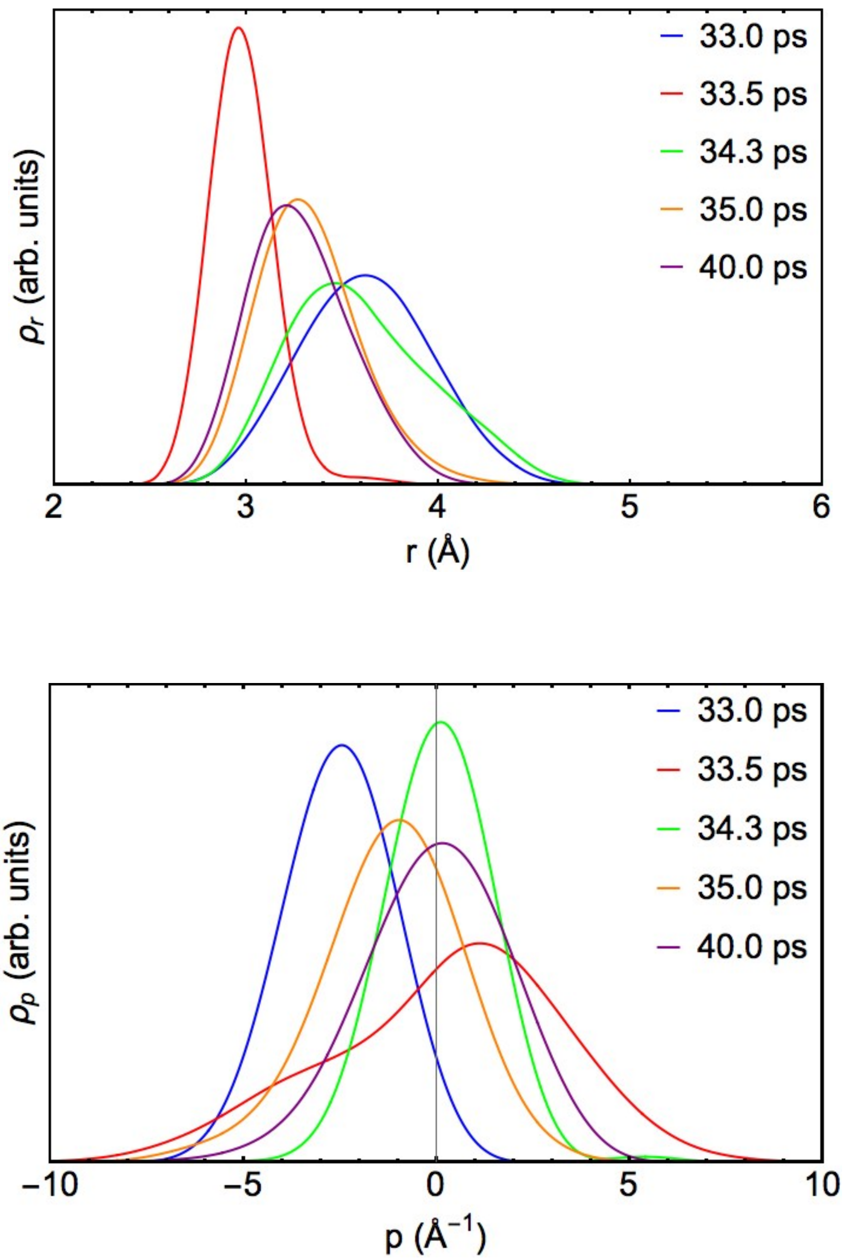

Figure S3. Snapshots showing the temporal evolution of the probability density of the relative coordinate wave packet in coordinate (up) and momentum (down) representations, for $<v_0>$=120 m/s and the nanodroplet with N=500.

Movie 1. Time evolution of the relative coordinate wave packet (squared modulus) in coordinate (in Å; up left) and momentum (in Å^{-1}, up right) representations. The effective potential energy is also plotted (in K; up left). Time evolution of the helium density in the xz-plane as 2D (down left) and 3D (down right) plots. This is for N=500, $\langle v_0 \rangle$=120 m/s and the simulated time is 71.0 ps. See the AVI video file "Movie 1_N500_v120.avi" (0.85 MB).

Movie 2. The same as Movie 1 but for N=500, $\langle v_0 \rangle$=500 m/s and the simulated time is 88.7 ps. See the AVI video file "Movie 2_N500_v500.avi" (1.00 MB).

Movie 3. The same as Movie 1 but for N=500, $\langle v_0 \rangle$=800 m/s and the simulated time is 31.7 ps. See the AVI video file "Movie 3_N500_v800.avi" (0.34 MB).

Movie 4. The same as Movie 1 but for N=200, $\langle v_0 \rangle$=120 m/s and the simulated time is 98.6 ps. See the AVI video file "Movie 4_N200_v120.avi" (1.13 MB).

Movie 5. The same as Movie 1 but for N=200, $\langle v_0 \rangle$=800 m/s and the simulated time is 48.9 ps. See the AVI video file "Movie 5_N200_v800.avi" (0.52 MB).

Movie 6. The same as Movie 1 but for N=1000, $\langle v_0 \rangle$=120 m/s and the simulated time is 65.2 ps. See the AVI video file "Movie 6_N1000_v120.avi" (0.77 MB).

Movie 7. The same as Movie 1 but for N=1000, $\langle v_0 \rangle$=800 m/s and the simulated time is 68.0 ps. See the AVI video file "Movie 7_N1000_v800.avi" (0.75 MB).