SUPPORTING INFORMATION

Quantum dynamics of the Br_2 (B-excited state) photodissociation in superfluid helium nanodroplets. Importance of the recombination process

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CONTENTS

Movie 1. Left up: time evolution of the Br_2(B) relative coordinate wave packet probability density (red) and the effective potential (black). Left down: time evolution of the Br_2(B) wave packet probability density in momentum representation. Right up: time evolution of the helium density in the xz-plane as a 2D plot. Right down: the same as the previous one but showing a 3D plot. The nanodroplet is formed by *N*=100 ^{4}He atoms.

Movie 2. As Movie 1 but for *N*=200 ^{4}He atoms.

Movie 3. As Movie 1 but for *N*=300 ^{4}He atoms.

Movie 4. As Movie 1 but for *N*=500 ^{4}He atoms.

Movie 5. As Movie 1 but for *N*=1000 ^{4}He atoms.

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Table s1. Cartesian grid parameters of helium, NIP and propagation time step. [a]

N	n_x	n_y	n_z	h_x (Å)	h_y (Å)	h_z (Å)	x_{min} (Å)	x_{max} (Å)	y_{min} (Å)	y_{max} (Å)	z_{min} (Å)	z_{max} (Å)
100	110	110	326	0.4	0.4	0.15	-22.0	21.6	-22.0	21.6	-24.45	24.30
200	120	120	386	"	"	"	-24.0	23.6	-24.0	23.6	-28.95	28.80
300	"	"	426	"	"	"	"	"	"	"	-31.95	31.80
500	130	130	454	"	"	"	-26.0	25.6	-26.0	25.6	-34.05	33.90
1000	190	190	520	"	"	"	-38.0	37.6	-38.0	37.6	-39.00	38.85

[a] Number of points (n_x,..), spatial separation (h_x,..) and minimum (x_{min},..)and maximum (x_{max},..) limits. Length of the NIP = 2.0 Å and A = 5171.4 K. Propagation time step (Δt) = 7.5 10^{-5} ps.

Table s2. Grid (r) of the Br_2(B) molecule, NIP and propagation time step.[a]

N	n_r	h_r (Å)	r_{min} (Å)	r_{max} (Å)	Δt (ps)
100	2418	1.796 10^{-2}	2.1	45.5	7.5 10^{-5}
200	2898	1.809 10^{-2}	"	54.5	"
300	3588	1.750 10^{-2}	"	69.6	"
500	3322	1.882 10^{-2}	"	64.6	"
1000	3928	1.882 10^{-2}	"	76.0	"

[a] Number of points (n_r), spatial separation (h_r) and minimum (r_{min}) and maximum (r_{max}) limits. Length of the NIP = 2.0 Å and A = 3315.0 K. Propagation time step (Δt) = 7.5 10^{-5} ps.

Table s3. Energy (E) contributions (in K) at t=0 for $Br_2(B)@(^4He)_N$ as a function of N. [a]

N	$E(He)_N$	E per atom of $(He)_N$	Kinetic E of $(He)_N$	Potential E of $(He)_N$
100	-118.5	-1.18	241.6	-449.1
200	-603.7	-3.02	282.0	-1007.2
300	-1130.2	-3.77	300.9	-1580.0
500	-2239.2	-4.48	325.6	-2773.9
1000	-5162.6	-5.16	370.3	-5922.1

N	Correlation E of $(He)_N$	Interaction E $Br_2(B) - (He$	Kinetic E $Br_2(B)$	Potential E $Br_2(B)$	Total E
100	89.0	-499.1	116.4	2016.8	1515.3
200	121.5	-514.2	116.4	2016.8	1015.3
300	148.9	-517.5	116.4	2016.8	485.5
500	209.1	-519.1	116.4	2016.8	-625.1
1000	389.1	-519.1	116.4	2016.8	-3548.5

[a] $E(He)_N$ corresponds exclusively to the total energy of helium that, according to the Orsay-Trento density functional, includes the following contributions: kinetic energy, potential energy (Lennard-Jones potential energy function) and correlation energy. The energy terms that refer exclusively to the diatomic molecule are the kinetic and the potential energy contributions. Finally, the total energy of the system is equal to the helium energy + molecule energy + helium-molecule interaction energy.

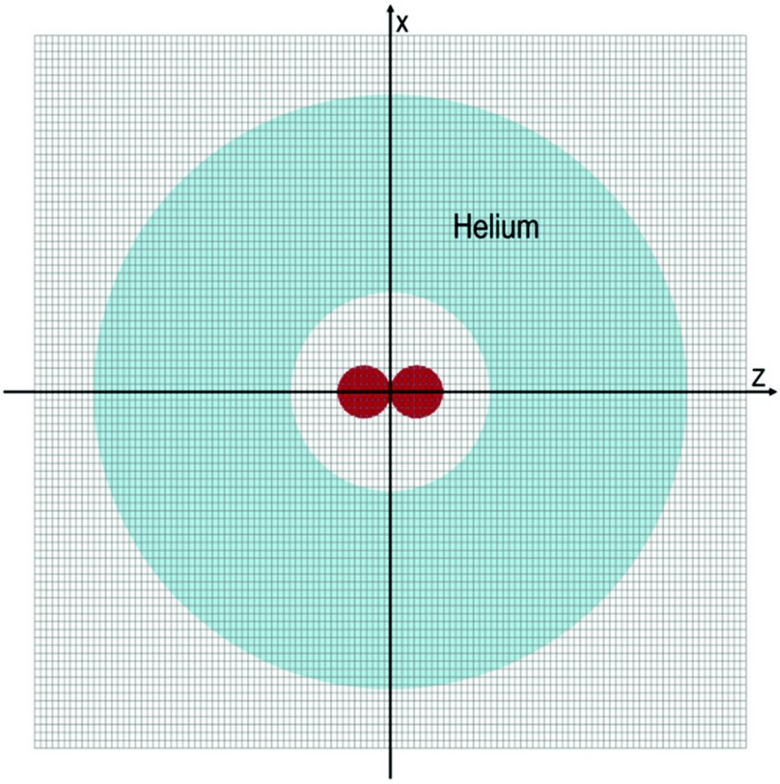

Figure s1. Schematic representation of the Cartesian grid used for the helium wave function (discretization in the xz plane). The blue zone corresponds to the region of the nanodroplet where the helium density takes non-negligible values and the red circles represent the diatomic molecule in the equilibrium geometry. Reproduced from ref. i with permission from the PCCP Owner Societies.

[i] M. Blancafort-Jorquera and M. González, Phys. Chem. Chem. Phys., 2021, **23**, 25961.