Supporting Information

Microscopic origin of quantum plasticity in small $H_3^+(H_2)_n$ (n = 1–3) clusters revealed by path integral molecular dynamics simulations

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Table S1. The Cartesian coordinates of the optimized structures of $H_3^+(H_2)_n$ (n = 1–3) clusters obtained by B3LYP+GD3/6-31G calculations.

Clusters	Atom	Coordinates [Å]		
		x	y	z
H_5^+ (C_{2v})	1	0.000000	0.000000	0.161655
	2	0.000000	0.400575	1.062336
	3	-0.000000	-0.400575	1.062336
	4	0.382253	-0.000000	-1.143163
	5	-0.382253	0.000000	-1.143163
H_5^+ (D_{2d})	1	0.000000	0.000000	0.000000
	2	0.000000	0.388792	1.065228
	3	-0.000000	-0.388792	1.065228
	4	0.388792	-0.000000	-1.065228
	5	-0.388792	0.000000	-1.065228
H_7^+ (C_{2v})	1	0.000000	0.000000	1.097513
	2	0.000000	0.483352	0.375772
	3	-0.000000	-0.483352	0.375772
	4	-0.377751	1.830169	-0.462264
	5	0.377751	1.830169	-0.462264
	6	0.377751	-1.830169	-0.462264
	7	-0.377751	-1.830169	-0.462264
H_9^+ (D_{3h})	1	0.000000	0.518778	0.000000
	2	0.449275	-0.259389	0.000000
	3	-0.449275	-0.259389	0.000000
	4	0.000000	2.200896	0.376385
	5	0.000000	2.200896	-0.376385
	6	1.906032	-1.100448	0.376385
	7	1.906032	-1.100448	-0.376385
	8	-1.906032	-1.100448	0.376385
	9	-1.906032	-1.100448	-0.376385

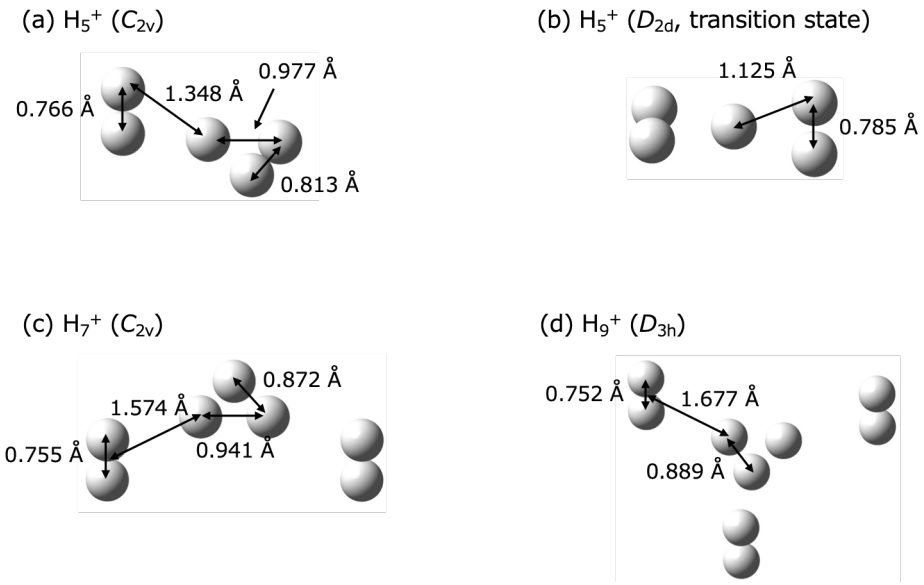

Figure S1. Optimized structures and representative interatomic distances [Å] of (a) H_5^+ (C_{2v}), (b) H_5^+ (D_{2d}, transition state), (c) H_7^+ (C_{2v}), and (d) H_9^+ (D_{3h}), obtained by static CCSD(T)/aug-cc-pVQZ calculations.

Table S2. Normal mode vectors (dimensionless) for modes 1, 2, 5, and 6 of H_7^+.

Mode	Atom	x	y	z	Mode	Atom	x	y	z
1	1	0.00	0.00	-0.00	5	1	0.00	-0.00	-0.00
	2	-0.01	0.00	-0.00		2	-0.01	0.00	-0.00
	3	0.01	-0.00	0.00		3	0.01	-0.00	-0.00
	4	-0.05	0.26	0.43		4	-0.08	0.42	-0.26
	5	-0.05	-0.26	-0.43		5	-0.08	-0.42	0.26
	6	0.05	-0.26	0.43		6	0.08	-0.42	-0.26
	7	0.05	0.26	-0.43		7	0.08	0.42	0.26
2	1	-0.25	-0.00	-0.00	6	1	0.23	-0.00	0.00
	2	-0.10	-0.00	-0.00		2	0.02	-0.00	0.00
	3	-0.10	-0.00	-0.00		3	0.02	-0.00	0.00
	4	0.11	0.29	0.37		4	-0.07	0.41	-0.26
	5	0.11	-0.29	-0.37		5	-0.07	-0.41	0.26
	6	0.11	0.29	-0.37		6	-0.07	0.41	0.26
	7	0.11	-0.29	0.37		7	-0.07	-0.41	-0.26